EMSP Communication Products

One of the goals of the EMSP is to focus the nation's science infrastructure on critical Department of Energy environmental problems. One of the "tried and true" ways to increase the general body of knowledge within the scientific community is through publication of research methods, results, and issues. EMSP research has provided a basis for numerous information exchanges through this method. EMSP researchers and staff have developed 1055 journal articles, papers, presentations, and other communication products. 115 articles have been submitted for review, and many additional news articles and press releases are either in development or planned as research within the program matures. The numbers of known publications and presentations as of March 30, 2000 are as follows:

- 358 Journal Articles
- 33 Other (Encyclopedias, manuscripts)
- 46 Papers
- 11 Patent disclosures and applications
- 19 Posters
- 424 Presentations
- 6 Press Releases
- 103 Proceeding Contributions
- 35 Reports
- 20 Theses/Dissertations

NOTE: In instances where an author was not identified for a particular communication product, the PI of the respective program has been listed as the author.

Project: 54122

Title: A Broad Spectrum Catalytic System for Removal of Toxic Organics from Water By Deep
PI: Dr. Ayusman Sen *Institution:* Pennsylvania State University

Publication Type: Journal

Chlistunoff, J. B. & Johnston, K. P. (1999). UV-Vis spectroscopic determination of the dissociation constant of bichromate from 160°C to 400°C. Journal of Phys. Chem. B. 102, 3993-4003.

Project: 54506

Title: Acid-Base Behavior in Hydrothermal Processing of Wastes
PI: Dr. Keith P. Johnston *Institution:* University of Texas at Austin

Publication Type: Journal

Chlistunoff, J. B., Ziegler, K. J., Lasdon, L., & Johnston, K. P. (1999). Nitric/nitrous acid equilibria in supercritical water. Journal of Phys. Chem. B. 103, 1678-1688.

Johnston, K. P. & Chlistunoff, J. B. (1998). Neutralization of acids and bases in subcritical and supercritical water: Acetic acid and HCl. Journal of Supercritical Fluids, 12, 155-64.

Ziegler, K. J., Lasdon, L., Chlistunoff, J., & Johnston, K. P. (1999, in press). Optimization models for determining nitric acid equilibria in supercritical water. Computers and Chemistry.

Publication Type: Report

Johnston, K. P. & Rossky, P. J. (1999, in press). Solution chemistry in supercritical water: spectroscopy and simulation. In E. Kiran (Ed.), NATO Adv. Study Institute on Supercritical Fluids.

Project: 54546

Title: Engineered Antibodies for Monitoring of Polynuclear Aromatic Hydrocarbons
PI: Dr. Alexander E. Karu *Institution:* University of California at Berkeley

Publication Type: Journal

Guo, F., Li, Q. X., & Alcantara-Licudine, J. P. (1999). A simple Na4 EDTA-assisted sub/supercritical fluid extraction procedure for quantitative recovery of polar analytes in soil. Anal. Chem. 71, 1309-1315.

Li, K., Chen, R., Zhao, B., Liu, M., Karu, A. E., Roberts, V. A., & Li, Q. X. (1999). Monoclonal antibody-based enzyme-linked immunosorbent assays for part-per-billion determination of polycyclic aromatic hydrocarbons: Effects of haptens and formats on sensitivity and specificity. Anal. Chem. 71, 302-309.

Liu, M., Li, Q. X, & Rechnitz, G. A. (1999). Flow injection immunosensing of polycyclic aromatic hydrocarbon with a quartz crystal microbalance. Analyt. Chim. Acta. 387, 29-38.

Liu, M., Li, Q. X, & Rechnitz, G. A. (1999, in press). Gold electrode modification with thiolated hapten for the design of amperometric and piezoelectric immunosensors. Electrochem. Anal.

Liu, M., Rechnitz, G. A., Li, K. & Li, Q. X. (1998). Capacitive immunosensing of polycyclic aromatic hydrocarbon and protein conjugates. Anal. Lett. 31, 2025-2038.

Publication Type: Poster

Karu, A. E., Li, Q. X., & Roberts, V. (1998, July 27-30). Engineered antibodies for monitoring of polynuclear aromatic hydrocarbons. Poster presented at Department of Energy Environmental Science Management Program Workshop. Chicago, IL. http: //www.osti.gov/em52/1998posters/id54546.pdf.

Publication Type: Presentation

Li, Q. X., Li, K., Thomas, S. & Li, H. (1999, Aug. 22-26). Application of immunochemical methods for the analysis of polynuclear aromatic hydrocarbons in the environment (Abstract No. NUCL0047). Symposium on First Accomplishments of the Environmental Management Science Program, 218th National Meeting of the American Chemical Society. New Orleans, LA.

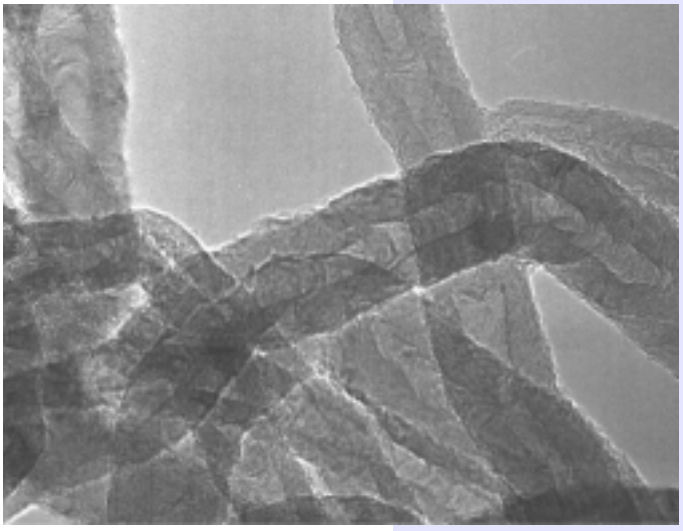
Pellequer, J.-L., Zhao, B., Kao, H.-I., Karu, A. E., & Roberts, V. A. (1999, Aug. 22-26). Cation-pi interactions in antibody binding of polynuclear aromatic hydrocarbons (Abstract No. 36750). Symposium on First Accomplishments of the Enviironmental Management Science Program, ACS Div. of Nuclear Chemistry and Technology, 218th National Meeting of the American Chemical Society. New Orleans, LA.

Project: 54571

Title: Removal of Heavy Metals and Organic Contaminants from Aqueous Streams by Novel Filtration Methods
PI: Dr. Nelly M. Rodriguez
Institution: Northeastern University

Publication Type: Journal

Anderson, P. E. & Rodriguez, N. M. (1999, in press). Growth of graphie nanofibers from the decomposition of CO/H2 over silica supported iron-nickel particles. J. Materials Research.



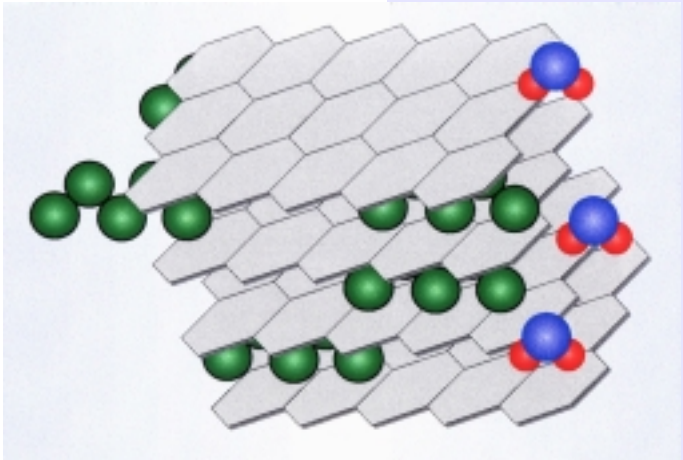
Transmission electron micrograph (TEM) of carbon nanofibers. [see Project #54571]

Project: 54576

Title: On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow
PI: Dr. William G. Gray
Institution: University of Notre Dame

Publication Type: Journal

Gray, W. G. (1999, in press). Macroscale equilibrium conditions for two-phase flow in porous media. International Journal of Multiphase Flow.



Organic impurity molecules being trapped between the graphene layers of a carbon nanofiber. Water molecules are preferentially absorbed at the edge sites of the structure. [see Project #54571]

Publication Type: Other

Soll, W. E., Gray, W. G. & Tompson, A. F. B. (1998). Influence of wettability on constitutive relations and its role in upscaling. In V. N. Burganos, et. al. (Eds.), Computational Methods in Water Resources XII, Computational Mechanics Publications, Southampton, Vol. 1, 413-420

Publication Type: Paper

Gray, W. G. (1999, Jan.). Thermodynamics and constitutive theory for multiphase porous-media flow considering internal geometric constraints. Advances in Water Resources, 22(5), 521-547.

Gray, W. G., & Hassanizadeh, S. M. (1998, July). Macroscale continuum mechanics for multiphase porous-media flow including phases, interfaces, common lines, and common points. Advances in Water Resources, 21(4), 261-281.

Muccino, J. C., Gray, W. G., & Ferrand, L. A. (1998, Aug.). Toward an improved understanding of multiphase flow in porous media. Reviews of Geophysics, 36(3), 401-422.

Project: 54585

Title: Permanganate Treatment of DNAPLs in Reactive Barriers and Source Zone Flooding Schemes

PI: Dr. Frank W. Schwartz *Institution:* Ohio State University

Publication Type: Journal

Yan, Y. E. & Schwartz, F. W. (1999). Oxidative degradation and kinetics of chlorinated ethylenes by potassium permanganate. Journal of Contaminant Hydrology. 37(3-4), 343-365.

Publication Type: Paper

Seol, Y. & Schwartz, F. W. (1999, Oct. 25-28). Phase transfer catalyst enhanced permanganate oxidation of trichloroethylene. Abstract for Annual conference of the Geological Society of America. Denver, CO.

Project: 54621

Title: Chemical Speciation of Strontium, Americium, and Curium in High Level Waste: Predictive Modeling of Phase Partitioning During Tank Processing

PI: Dr. Andrew R. Felmy *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Felmy, A. R. & Mason, M. J. (1998). The displacement of strontium from organic chelates by hydroxide, carbonate, and calcium in concentrated electrolytes. Journal of Solution Chemistry, 27(5), 435-454.

Felmy, A. R. & Rai, D. (1999, in press). Application of Pitzer's equations for modeling the aqueous thermodynamics of actinide species: A review. Invited paper for the special memorial edition of the Journal of Solution Chemistry in honor of Professor Kenneth Pitzer.

Felmy, A. R., Dixon, D. A., Rustad, J. R., Mason, M. J. & Onishi, L. M. (1998). The hydrolysis and carbonate complexation of strontium and calcium in aqueous electrolytes: Use of molecular modeling calculations in the development of aqueous thermodynamic models. Journal of Chemical Thermodynamics 30, 1103-1120.

Oakes, C. S., Sterner, S. M. & Felmy, A. R. (1999, in press). Thermodynamic properties of aqueous calcium nitrate [Ca(NO3)2] to 373K including new enthalpy of dilution data. Journal of Chemical Thermodynamics.

Sterner, S. M., Felmy, A. R., Oakes, C. S., & Pitzer, K. S. (1998). Correlation of thermodynamic data for aqueous electrolyte solutions to very high ionic strength using INSIGHT: Vapor saturated water activity in the system CaCl2-H2O to 250 ° C and solid saturation. International Journal of Thermophysics, 193, 761-770.

Publication Type: Presentation

Felmy, A. R., Choppin, G. R., Dixon, D. A., & Campbell, J. A. (1998, Jul. 27-30). Chemical speciation of strontium, americium, and curium in high-level waste: Predictive modeling of phase partitioning during tank processing. Two presentations and one poster. Presentations to the Hanford Tanks Site Technology Coordination Group (STCG) on November 10, 1998, and to PNNL staff on January 21, 1998. Poster presentation at the EMSP Principal Investigators Workshop, Chicago, IL.

Felmy, A. R. & Mason, M. J. (1998, Aug. 9-14). The aqueous complexation of Eu(III) with organic chelating agents at high base and high ionic strengths: Metal-chelate displacement induced by hydrolysis and precipitation reactions. 53rd Calorimetry Conference. Midland, MI.

Felmy, A. R., Dixon, D. A. & Mason, M. J. (1997, Aug. 3-8). The complexation of alkaline earth cations by organic chelates at high ionic strength: Competitive effects of hydrolysis and carbonate complextion. 52nd Calorimetry Conference. Asilomar, CA.

Felmy, A. R., Dixon, D. A. & Mason, M. J. (1999, Mar. 21-25). Aqueous complexation of Eu(III) with organic chelating agents at high base concentration: Molecular and thermodynamic modeling results. 217th ACS National Meeting. Anaheim CA.

Felmy, A. R., Dixon, D. A., Campbell, J. A. & Mason, M. J. (1997, Sept. 7-11). The effects of OH, CO3, and Ca on the displacement of strontium from organic chelates: Implications for waste processing. 214th ACS National Meeting. Las Vegas, NV.

Felmy, A. R., Dixon, D. A., Rustad, J. R., Mason, M. J. & Onishi, L. M. (1997, Aug. 3-8). The use of molecular modeling calculations to improve the development of thermodynamic models: Hydrolysis, carbonate, and EDTA complexation of alkaline earth cations. 52nd Calorimetry Conference. Asilomar, CA.

Oakes, C. S. & Felmy, A. R. (1997, Aug. 3-8). Thermodynamics of [Na4EDTA+NaOH]{aq}, including new isopiestic measurements, to 373K, 0.1MPa, and stoichiometric ionic strengths of 18 . 9mol . kg -1. 52nd Calorimetry Conference, Asilomar, CA.

Oakes, C. S. & Felmy, A. R. (1998, Aug. 9-14). Thermodynamics of [Na4EDTA+NaOH]{aq}, including new isopiestic and enthalpy of dilution measurements. 53rd Calorimetry Conference. Midland, MI.

Petersen, C. E., Campbell, J. A., Felmy, A. R., Wahl, K. L. & Finch, J. W. (1998, May 31-June 4). Analysis of metal-organic complexes using CE/MS. 46th American Society of Mass Spectrometry Meeting. Orlando, FL.

Sterner, S. M., Felmy, A. R. & Pitzer, K. S. (1997, Jun. 22-27). Correlation of thermodynamic data for aqueous electrolyte solutions to very high ionic strength using INSIGHT: Vapor saturated water activity in the system CaCl2-H2O to 250 ° C and solid saturation. Thirteenth Symposium on Thermophysical Properties. Boulder, CO.

Sterner, S. M., Felmy, A. R., Oakes, C. S., Simonson, J. M., & Pitzer, K. (1997, Aug. 3-8). Thermodynamics of aqueous CaCl2 to 250 ° C, 400 bars and solid saturation. 52nd Calorimetry Conference. Asilomar, CA.

Project: 54628

Title: Colloidal Agglomerates in Tank Sludge: Impact on Waste Processing
PI: Dr. Joel M. Tingey *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Tingey, J. M., Bredt, P. R., & Shekarriz, R. (1999, Mar.). Rheology and settling behavior of Hanford tank wastes and the resulting process streams. Rheology in Mineral Industry II. Kahuku, Oahu, HI.

Tingey, J. M., Bunker, B. C., Graff, G. L., Keefer, K. D., Lea, A. S., & Rector, D. R. (1998, Nov.). Colloidal agglomerates in tank sludge and their impact on waste processing. Materials Research Society Fall Meeting. Boston, MA.

Tingey, J. M., Graff, G. L., & Rector, D. R. (1999, Mar.). Effect of colloidal aggregation on sedimentation and rheology in highly basic, high ionic strength salt solutions. Rheology in Mineral Industry II. Kahuku, Oahu, HI.

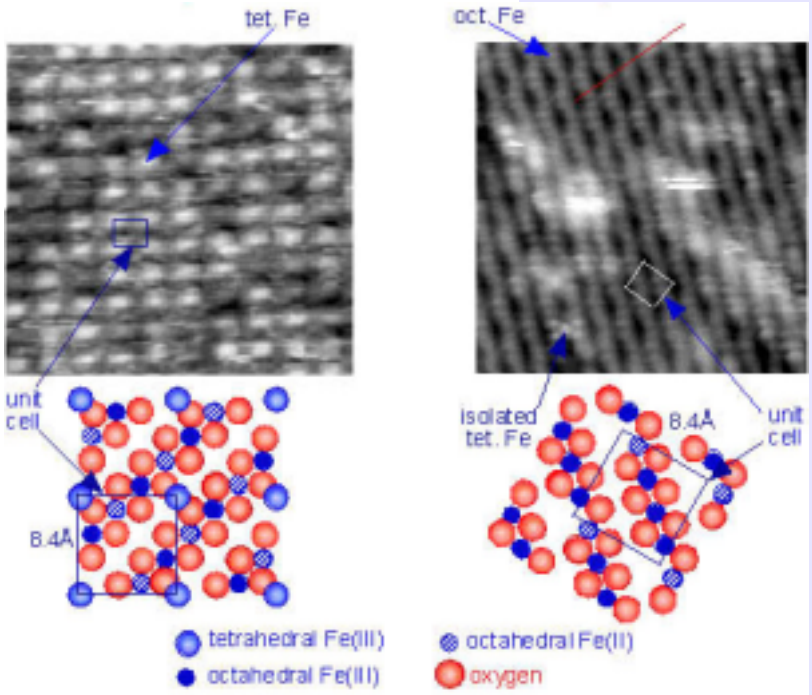
Project: 54635

Title: Molecular-Level Process Governing the Interaction of Contaminants with Iron and Manganese

PI: Dr. Scott A. Chambers

Institution: Pacific Northwest National Laboratory

Publication Type: Journal



Left: Top layer consists of tetrahedrally coordinated Fe(III), as shown in the structural diagram. Right: Top layers consist of octahedrally coordinated Fe(II) and Fe(III), along with tetrahedrally coordinated O, as shown in the structural diagram. [see Project #54635]

Brown, G. E. Jr., et. al. (1999). Metal oxide surfaces and their interactions with aqueous solutions and microbial organisms. Chem. Rev. 99, 77-174.

Chambers, S. A. & Liang, Y. (1999). Growth of • -MnO2 films on TiO2(110) by oxygen-plasma-assisted molecular beam epitaxy. Surf. Sci. Spect. 420, 123.

Chambers, S. A., & Joyce, S. A. (1999). Surface termination, composition, and reconstruction of Fe3O4(001) and • -Fe2O3(001). Surf. Sci. Spect. 420, 111.

Chambers, S. A., Gao, Y. & Kim, Y. J. (1998). Fe 2p core-level spectra for pure, epitaxial • -Fe2O3(0001), • -Fe2O3(001), and Fe3O4(001). Surf. Sci. Spect. 5, 219.

Foster, N. S., Amonette, J. E., & Autrey, S. T. (1999, in press). In-situ detection of chromate using photoacoustic spectroscopy. Appl. Spectrosc.

Foster, N. S., Autrey, S. T., Amonette, J. E., Small, J. R., & Small, E. W. (1999). Laser photoacoustic spectroscopy: A versatile absorption spectroscopic technique. Am. Lab. 31, 96s-108s.

Grolimund, D., et. al. (1999, in press). Identification of Cr species at the aqueous solution hematite interface after Cr(VI)-Cr(III) reduction using GI-XAFS and Cr L-edge NEXAFS. Journal of Synchrotron Radiation.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1999). Reaction of water with the (100) and (111) surfaces of Fe3O4." Surface Science.

Kendelewicz, T., Liu, P., Doyle, C. S., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1999). "X-ray absorption and photoemission study of the adsorption of aqueous Cr(VI) on single crystal hematite and magnetite surfaces." Surf. Sci. Spect. 424, 219.

Liu, P., Kendelewicz, T., Brown, G. E. Jr., Nelson, E. J. & Chambers, S. A. (1998). Reaction of water vapor with • -Al2O3(0001) and • -Fe2O3(0001) surfaces: Synchrotron x-ray photoemission studies and thermodynamic calculations." Surf. Sci. Spect. 417, 53.

Rustad, J. R., Dixon, D. A., Kubicki, J. D., & Felmy, A. R. (1999, in press). Gas-phase acidities of tetrahedral oxyacids from ab initio electronic structure calculations. J. Phys. Chem.

Rustad, J. R., Wasserman, E., & Felmy, A. R. (1999, in press). A molecular dynamics investigation of surfacereconstruction on magnetite (001)." Surf. Sci. Spect.

Thevuthasan, S., et. al. (1999). Surface structure of MBE-grown • -Fe2O3(0001) by intermediate-energy x-ray photoelectron diffraction. Surf. Sci. Spect. 425, 276-286.

Yi, S. I., Liang, Y. & Chambers, S. A. (1999). Effect of growth rate on the nucleation of • -Fe2O3 on • -Al2O3(0001) by oxygen-plasma-assisted molecular beam epitaxy. J. Vac. Sci. Technol. A.

Publication Type: Presentation

Amonette, J. E., Foster, N. S., William, B. K., & Taylor, A. E. (1999, Mar. 21-25). Trace-level chromate sorption dynamics at hematite surfaces: A spectroscopic approach. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Amonette, J. E., Foster, N. S., William, B. K., & Taylor, A. E. (1999, Jun.). Competitive trace-level sorption of chromate and phosphate to hematite surfaces: A spectroscopic approach. 36th Annual Meeting of the Clay Minerals Society. Purdue University. West Lafayette, IN.

Brown, G. E. Jr., et. al. (1999, Mar.). Characterization of adsorbed chemical species at mineral surfaces. 217th American Chemical Society Meeting. Anaheim, CA.

Chambers, S. A. (1998, Oct.). Molecular beam epitaxial growth and surface structure determination of Fe and Mn oxides. Invited presentation at the Center for Catalysis and Surface Structure. Northwestern University. Evanston, IL.

Chambers, S. A., Thevuthasan, S., Kim, Y. J., Joyce, S. A., & Liang, Y. (1998, Aug.). Surface structure determination of MBE grown iron and manganese oxides. Invited presentation at the National Meeting of the American Chemical Society. Boston, MA.

Chambers, S. A.,Thevuthasan, S., & Joyce, S. A. (1999, Jan.). Structure and reactivity of MBE-grown Fe oxides. Invited presentation at the First International Conference on Oxide Surfaces. Elmau, Germany.

Grolimund, D., et. al. (1998, Jul.). Identification of Cr species at the solution-hematite interface after Cr(VI)-Cr(III) reduction using GI-XAFS and Cr L-edge NEXAFS. 10th International XAFS Conference. Chicago, IL.

Grolimund, D., Fitts, J. P., Trainor, T. P., Brown, G. E. Jr., & Chambers, S. A. (1999, Mar.). Identification of Cr species at the aqueous solution-oxide interface using grazing-incidence XAFS. 217th American Chemical Society Meeting. Anaheim, CA.

Joyce, S. A., Thevuthasan, S., & Chambers, S. A. (1999, Mar. 21-25). Growth and structure of synthetic iron oxide mineral surfaces. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., & Nelson, E. J. (1998, Aug.). Reaction of water with (100) and (111) surfaces of magnetite (Fe3O4). International Conference on Surface Science 10. Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Chambers, S. A., & McCarthy, M. I. (1998, Aug.). “Hydroxylation of the surfaces of simple metal oxides: Spectroscopic and thermodynamic analysis. Goldschmidt Conference. Toulouse, France.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Reduction of the (0001) surface of hematite (• -Fe2O3) prepared under UHV conditions. International Conference on Surface Science 10. Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Fe L2,3 and O K near edge structure of iron oxides and hydroxides. International Conference on Surface Science 10.Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Reaction of water with clean (0001) and (1-102) surfaces of • -Fe2O3. International Conference on Surface Science 10. Birmingham, United Kingdom.

McCready, D. E., (1998, Jun.). Rutherford backscattering and channeling studies of epitaxially grown iron oxide films on various substrates. Surface Analysis/8th Annual Pacific Northwest Symposium.

Rustad, J. R. (1999, Aug.). Molecular simulation of the iron oxide-water interface. Invited presentation at the American Chemical Society Meeting. New Orleans, LA.

Rustad, J. R., Wasserman, E., & Joyce, S. A. (1999, Mar. 21-25). Structure and energetics of the magnetite(001) surface insights from molecular dynamics calculations. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Thevuthasan S. (1998, Nov.). Rutherford backscattering and channeling studies of Al and Mg diffusion in iron oxide thin films. Invited presentation at the Fifteenth International Conference on the Application of Accelerators. Denton, TX.

Thevuthasan, S., et. al. (1998, Jun.). The surface structure determination of • -Fe2O3 by intermediate-energy x-ray photoelectron diffraction. Surface Analysis/8th Annual Pacific Northwest Symposium.

Thevuthasan, S., et. al. (1998, Nov.). The surface structure determination of • -Fe2O3 (0001) by low-energy x-ray photoelectron diffraction. 45th National Symposium of the American Vacuum Society.

Thevuthasan, S., Jiang, W., McCready, D. E., & Chambers, S. A. (1998, Nov.). Rutherford backscattering and channeling studies of Al and Mg diffusion in iron oxide thin films. 45th National Symposium of the American Vacuum Society.

Thevuthasan, S., McCready, D. E., Jiang, W., Yi, S. I., & Chambers, S. A. (1999, Jul.). Ion beam analysis of interface reactions in iron oxide thin films. Invited presentation at the Fourteenth International Conference on Ion Beam Analysis (IBA-14). Dresden, Germany.

Publication Type: Proceeding

Chambers, S. A., & Liang, Y. (1998, Nov.). Growth of • -MnO2 films on TiO2(110) by oxygen-plasma- assisted molecular beam epitaxy." 45th International Symposium of the American Vacuum Society. Baltimore, MD.

Project: 54639

Title: Development of an In-Situ Microsensor for the Measurements of Chromium and Uranium in Groundwater at DOE Sites

PI: Dr. Joseph Wang *Institution:* New Mexico State University

Publication Type: Journal

Wang, J., Bhada, R., Lu, J., & MacDonald, D. (1998). Remote sensor for monitoring TNT in natural waters. Anal. Chim. Acta, 361, 85.

Wang, J., Lu, J., & Augelli, M. (1999). In-situ flow probe for improving the performance of electrochemical stripping analysis. Fres. J. Anal. Chem., 364, 28.

Wang, J., Lu, J., Tian, B., MacDonald, D., & Olsen, K. (1999). Flow probe for in-situ electrochemical monitoring of trace chromium. Analyst, 124, 349.

Wang, J., Tian, B., & Lu, J. (1998). Electrochemical flow sensor for in-situ monitoring of total metal concentration. Anal. Communications, 35, 241.

Wang, J., Tian, B., Lu, J., & MacDonald, D. (1998). Remote electrochemical sensor for monitoring trace mercury. Electroanalysis 10, 399.

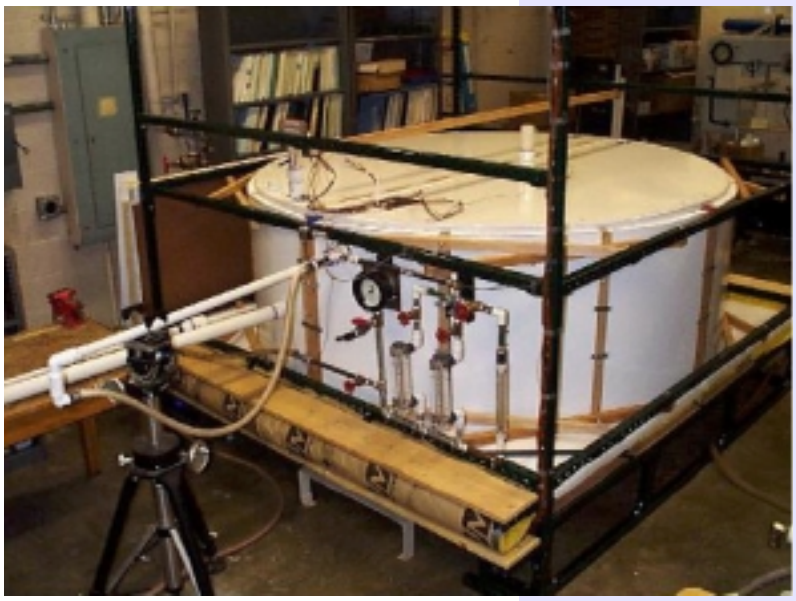
Wang, J., Tian, B., Lu, J., Yarnitsky, C., Olsen, K., & Bennet, W. (1999). Stripping analysis into the 21st century: Faster, smaller, simpler, and better. Anal. Chim. Acta, 385, 429.

Project: 54656

Title: Mixing Processes in High-Level Waste Tanks
PI: Dr. Per F. Peterson
Institution: University of California at Berkeley

Publication Type: Presentation

Christensen, J. & Peterson, P. F. (1999, Oct. 3-8). A one-dimensional lagrangian model for large-volume mixing. Accepted for the Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics. San Francisco, CA.



Study of Mixing and heat-transfer augmentation by injected jets in a large enclosure. [see Project #54656]

Kuhn, S. Z., Lee, C., & Peterson, P. F. (1999, Oct. 3-8). "Stratification from buoyancy-driven exchange flow through horizontal partitions in a liquid tank. Accepted for the Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics. San Francisco, CA.

Publication Type: Proceeding

Peterson, P. F. & Gamble, R. E. (1998). Scaling for forced-convection augmentation of heat and mass transfer in large enclosures by injected jets. Transactions of American Nuclear Society, 78, 265-266.

Project: 54666

Title: Mechanisms, Chemistry, and Kinetics of Anaerobic Biodegradation of cDCE and Vinyl Chloride
PI: Dr. Perry L. McCarty *Institution:* Stanford University

Publication Type: Journal

Haston, Z. C. & McCarty, P. L. (1999). Chlorinated ethene half-velocity coefficients (K S) for reductive dehalogenation. Environmental Science and Technology, 33(2), 223-226.

Rosner, B., McCarty, P. L., & Spormann, A. M. (1997). In vitro studies on reductive vinyl chloride dehalogenation by an anaerobic mixed culture. Appl. Environ. Microbiol., 63 (11): 4139-4144.

Yang, Y. & McCarty, P. L. (1998). Competition for hydrogen within a chlorinated solvent dehalogenating mixed culture. Environmental Science and Technology, 32(22), 3591-3597.

Yang, Y. & McCarty, P. L. (1999, in press). Response to "Comment on competition for hydrogen within a chlorinated solvent dehalogenating anaerobic mixed culture." Environmental Science & Technology.

Project: 54672

Title: Radiation Effects in Nuclear Waste Materials
PI: Dr. William J. Weber *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Gorretta, K. C., et. al. (1999). Solid-particle erosion of Portland cement and concrete. Wear 224, 106-112.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). U and Pu LIII XAFS of Pu-doped glass and ceramic waste forms. Journal of Alloys and Compounds, 271-273, 240-243.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. Journal of Nuclear Materials, 254: 175-184.

Weber, W. J., Ewing, R. C., & Meldrum, A. (1997). The kinetics of alpha-decay-induced amorphization in zircon and apatite containing weapons-grade plutonium or other actinides. Journal of Nuclear Materials, 250, 147-155.

Williford, R. E., Devanathan, R., & Weber, W. J. (1998). Computer simulation of displacement threshold energies for several ceramic materials. Nuclear Instruments and Methods B 141, 98-103.

Williford, R. E., Weber, W. J., Devanathan, R., & Cormack, A. N. (1999, in press). Native vacancy migrations in zircon. Journal of Nuclear Materials.

Publication Type: Other

Begg, B. D., et. al. (1999, in press). Heavy-ion irradiation effects in pyrochlores. In Smith, G. L., Chandler, G. T., & Mobasher, B. (Eds.), Waste Management Science and Technology in the Ceramic andNuclear Industries. The American Ceramic Society. Westerville, OH.

Chen, X. & Birtcher, R. C. (1999, in press). Bubble formation and growth in nuclear waste glasses. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.). Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540. Warrendale, PA.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, in press). Vacancy migration and excitons in silica polymorphs. In Smith, G. L., Chandler, G. T., & Mobasher, B. (Eds.). Mater. Waste Management Science and Technology in the Ceramic and Nuclear Industries. The American Ceramic Society. Westerville, OH.

Publication Type: Paper

Williford, R. E. & Weber, W. J. (1999, Apr. 25-28). Defect formation and migration energetics in disordered Gd2Ti2O7. The 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Publication Type: Presentation

Begg, B. D., et. al. (1999, Apr. 25-28). Heavy-ion irradiation effects in pyrochlores. The 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Begg, B. D., Hess, N. J., & Weber, W. J. (1999, Apr. 22-23). XAS and XRD characterization of annealed Pu-doped zircon. CEA Meeting on HLW and Pu Immobilization. Saclay, France.

Chen, X., Birtcher, R. C., & Donnelly, S. E. (1998, Nov. 30 - Dec. 4). Bubble formation and growth in nuclear waste glasses. Materials Research Society Annual Meeting. Boston, MA.

Corrales, L. R. & Song, J. (1997, Sept.). Molecular dynamics simulations of excitons in glasses. CEA/VALHRO Summer School. Mejannes le Clap, France.

Corrales, L. R. (1997, Oct.). Lattice theories and molecular dynamics simulations of glasses. Department of Chemistry, University of Maryland. College Park, MD.

Corrales, L. R. (1997, Oct.). Molecular dynamics simulations of defects and excitons in glasses. American Ceramics Society, Glass and Optical Materials Division Meeting. Williamsburg, VA.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, Apr. 25-28). The formation and migration energetics of radical defects in silica polymorphs. Invited presentation at the 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, Mar. 21-25). Migration of oxygen vacancy radical defects and self-trapped excitons in silica. Invited presentation at the 217th American Chemical Society Meeting. Anaheim, CA.

Corrales, L. R., VanGinhoven, R. M., Song, J., & Jónsson, H. (1998, Nov. 30 - Dec. 4). Vacancy migration barrier energetics and pathways in silica. Materials Research Society Annual Meeting. Boston, MA.

Devanathan, R., Weber, W. J., & Boatner, L. A. (1997, Dec. 1-5). Response of zircon to electron and Ne + irradiation. Materials Research Society Annual Meeting. Boston, MA.

Devanathan, R., Weber, W. J., & Williford, R. E. (1998, Nov. 30 - Dec. 4). Amorphization of Gd2Ti2O7 by energetic heavy ion irradiation. Materials Research Society Annual Meeting. Boston, MA.

Fortner, J. A., Hanchar, J. M., Badyal, Y., Price, D. L., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Structural analysis of a completely amorphous 238 Pu-doped zircon by neutron diffraction. Materials Research Society Annual Meeting. Boston, MA.

Hess, N. J., Maupin, G. D., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Spectroscopic studies of gamma-irradiated glass waste forms. Materials Research Society Annual Meeting, Boston, MA.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1997, Sept. 21-26). U and Pu LIII XAFS of Pu-doped glass and ceramic waste forms. International Conference on Actinides ‘97. Baden-Baden, Germany.

Song, J. & Corrales L. R. (1998, Mar. 16-20). Simulation of exciton processes in networked materials. March APS National Meeting. Anaheim, CA.

Song, J., Corrales, L. R., & Jónsson, H. (1998, Nov. 30 - Dec. 4). Exploring the excited states of vacancy defects in silica. Materials Research Society Annual Meetin. Boston, MA.

Thevuthasan, S., Jiang, W., McCready, D. E., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Damage accumulation and thermal recovery in SrTiO3 implanted with various ions. Materials Research Society Annual Meeting. Boston, MA.

Weber, W. J. & Corrales, L. R. (1998, July 27-30). Radiation effects in nuclear waste forms. DOE Environmental Management Science Program Scientific Workshop. Rosemont, IL.

Weber, W. J. & Devanathan, R. (1998, May 4-6). Effects of alpha decay on crystalline ceramic waste forms. American Ceramic Society Meeting. Cincinnati, OH.

Weber, W. J. (1988, July 27-30). EMSP projects in materials science. DOE Environmental Management Science Program Scientific Workshop. Rosemont, IL.

Weber, W. J. (1997, Dec. 1). Radiation effects in glass and ceramic waste forms. Invited presentation at the Massachusetts Institute of Technology. Cambridge, MA.

Weber, W. J. (1997, Dec. 11). Radiation effects in glass waste forms. Invited presentation at Argonne National Laboratory. Argonne, IL.

Weber, W. J. (1997, Feb. 20). Radiation effects from the incorporation of plutonium in glasses and ceramics. Invited presentation at Los Alamos National Laboratory. Los Alamos, NM.

Weber, W. J. (1998, Apr. 19-22). Effects of radiation on solid nuclear waste forms. Invited plenary lecture at the DOE Workshop on Research Needs and Opportunities in Radiation Chemistry. Chesterton, IN.

Weber, W. J. (1998, Apr. 3-4). Radiation effects from alpha decay in nuclear waste ceramics. Invited plenary lecture at the American Nuclear Society Northern Student Conference. Ann Arbor, MI.

Weber, W. J. (1998, Jan. 8). Radiation effects in crystalline waste form phases. Invited presentation at the Idaho National Engineering and Environmental Laboratory. Idaho Falls, ID.

Weber, W. J., et. al. (1998, Nov. 30 - Dec. 4). The effect of temperature and recoil spectra on amorphization in zircon. Materials Research Society Annual Meeting. Boston, MA.

Weber, W. J., Ewing, R. C., & Meldrum, A. (1998, Mar. 30 - Apr. 3). Radiation effects in nuclear waste ceramics. American Chemical Society Annual Meeting. Dallas, TX.

Weber, W. J., Hess, N. J., Conradson, S. D., & Vienna, J. D. (1997, Aug. 25-27). Self-radiation effects in glass and ceramic waste forms for the stabilization and disposition of plutonium. Topical Conference onPlutonium Futures - The Science. Santa Fe, NM.

Williford, R. E., Devanathan, R. & Weber, W. J. (1997, Sept. 14-19). Computer simulation of displacement threshold energies for several ceramic materials. 9th International Conference on Radiation Effects in Insulators. Knoxville, TN.

Williford, R. E., Weber, W. J., Devanathan, R., & Gale, J. D. (1998, Nov. 30 - Dec. 4). Oxygen vacancy migration in Gd2(Ti,Zr)2O7 pyrochlores. Materials Research Society Annual Meeting. Boston, MA.

Publication Type: Proceeding

Begg, B. D., Hess, N. J., & Weber, W. J. (1999, in press). XAS and XRD characterization of annealed Pu-doped zircon. In Meis, C. & Carpena, J. (Eds.), Proceedings of the CEA Meeting on HLW and Pu Immobilization, CEA/Saclay.

Corrales, L. R. & Song, J. (1998). Semi-empirical methodology to simulate exciton processes in glasses. Proceeds of the CEA/VALRHO Summer School on Glass: Scientific Research for High Performance Containment. CEA/Valrhô, Bagnols-sur-Cèze, France, 218-227.

Corrales, L. R., VanGinhoven, R. M., Song, J., & Jónsson, H. (1999). Vacancy migration barrier energetics and pathways in silica. In Bulatov, V. V., Diaz de la Rubia, T., Phillips, R., Kaxiras, E., & Ghoniem, N. (Eds.) Multiscale Modeling of Materials. Mater. Res. Soc. Symp. Proc. 538, Warrendale, PA. 317-321.

Devanathan, R., Weber, W. J., & Boatner, L. A.. (1998). Response of zircon to electron and Ne + irradiation. In Ma, E., Bellon, P., Atzmon, M., & Trivedi, R. (Eds.) Phase Transformations and Systems Driven far from Equilibrium. Mater. Res. Soc. Symp. Proc. 481, Warrendale, PA. 419-424.

Fortner, J. A., Hanchar, J. M., Badyal, Y., Price, D. L., & Weber, W. J. (1999, in press). Structural analysis of a completely amorphous 238 Pu-doped zircon by neutron diffraction. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.). Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Heinisch, H. L., Williford, R. E. & Weber, W. J. (1998, Nov. 30 - Dec. 4). Computer simulations of irradiation-induced defect accumulation and amorphization in zircon. Materials Research Society Annual Meeting. Boston, MA.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1997, Sept. 28 - Oct. 3). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. MRS Symposium, Scientific Basis for Nuclear Waste Management XXI. Davos, Switzerland.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. In McKinley, I. G. & McCombie, C. (Eds.), Scientific Basis for Nuclear Waste Management XXI. Mater. Res. Soc. Symp. Proc. 506, Warrendale, PA. 169-176.

Thevuthasan, S., Jiang, W., McCready, D. E., & Weber, W. J. (1999, in press). Damage accumulation and thermal recovery in SrTiO3 implanted with various ions. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Weber, W. J., et. al. (1999, in press). The effect of temperature and recoil spectra on amorphization in zircon. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Publication Type: Report

Weber, W. J., Hess, N. J., Conradson, S. D., & Vienna, J. D. (1997). Self-radiation effects in glass and ceramic waste forms for the stabilization and disposition of plutonium. Plutonium Futures - The Science. LA-13338-C, Los Alamos National Laboratory. Los Alamos, NM. 25-26.

Weber, W. J. & Corrales, L. R. (1997). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. PNNL-11589, Pacific Northwest National Laboratory. Richland, WA. 43-52.

Weber, W. J. & Corrales, L. R. (1998). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. PNNL-11889, Pacific Northwest National Laboratory. Richland, WA. 1.107-1.126.

Project: 54679

Title: Architectural Design Criteria for F-Block Metal Ion Sequestering Agents
PI: Dr. Benjamin P. Hay *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Clement, O., Rapko, B. M., & Hay, B. P. (1998). Structural aspects of metal-amide complexes. Coordination Chemistry Reviews 170, 203.

Falana, O. M., Koch, H. R., Roundhill, D. M., Lumetta, G. J., & Hay, B. P. (1998). Synthesis and extraction studies of 1,2- and 1,3-disubstituted butylcalix[4]Arene amides with oxyions: Geometric and conformational effects. Journal of the Chemical Society, Chemical Communications 503.

Hay, B. P., Clement, O., Sandrone, G., & Dixon, D. A. (1998). A MM3(96) force field for metal amide complexes. Inorganic Chemistry, 37, 5887.

Lumetta, G. L., McNamara, B. K., & Rapko, B. M. (1999, in press). Complexation of uranyl ion by tetrahexyl-malonamides: An equilibrium modeling and infrared spectroscopic study. Inorganica Chimica Acta.

McNamara, B. K., Lumetta, G. J. & Rapko, B. M. (1999, in press). Extraction of europium(III) ion with tetrahexylmalonamides. Solvent Extraction and Ion Exchange.

Rao, L., Xia, Y., Rapko, B. M., & Martin, P. F. (1998). Synergistic extraction of Eu(III) and Am(III) by thenoyltrifluoroacetone and neutral donor extractants: Octyl(phenyl)-N,N-diisobutylcarbonyl-methylphosphine oxide and 2,6-bis(diphenylphosphino)methyl pyridine N,P,P trioxide. Solvent Extraction and Ion Exchange, 16, 913.

Rapko, B. M., McNamara, B. K., Lumetta, G. J., Rogers, R. D., & Hay, B. P. (1999, in press). Coordination chemistry of lanthanide nitrates with N,N,N,N-tetramethylsuccinamide. Inorganic Chemistry.

Sandrone, G., Dixon, D. A., & Hay, B. P. (1999). C(sp 2)-C(sp 3) rotational barriers in simple amides: H2N-C(=O)-R, R = methyl, ethyl, i-propyl, t-butyl. Journal of Physical Chemistry, A 103, 893.

Sandrone, G., Dixon, D. A., & Hay, B. P. (1999). Conformational analysis of malonamide, N,N'-dimethylmalonamide, and N,N,N',N'-tetramethylmalonamide. Journal of Physical Chemistry, A.18: 3554

Wolf, N. J., et. al. (1999, in press). Synthesis of lower rim amine and carbamoyl substituted calixarenes as transfer agents for oxyions between an aqueous and a chloroform phase. Polyhedron.

Yordanov, A. & Roundhill, D. M. (1998). Solution extraction of transition and post-heavy and precious metals by chelate and macrocyclic ligands. Coordination Chemistry Reviews, 170, 93.

Yordanov, A. T., et. al. (1999). Derivatized calix[4]arenes as selective phase transfer extractants for heavy metal and oxyion salts. Comments on Inorganic Chemistry, 20, 163.

Publication Type: Other

Hay, B. P. & Clement, O. (1998). Metal complexes. Invited Book Chapter In Schleyer, P. R., et. al. (Eds.) The Encyclopedia of Computational Chemistry. John Wiley and Sons, Chichester, NY.

Publication Type: Presentation

Clement, O., Hay, B. P. Dixon, D. A., & Sandrone, G. (1998, Jun.). A MM3(96) force field for metal-amide complexes. West Coast Theoretical Chemistry Conference. Richland, WA.

Clement, O., Sandrone, G., Dixon, D. A., & Hay, B. P. (1998, Jun.). A MM3(96) force field for metal-amide complexes. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Clement, O., Sandrone, G., Dixon, D. A., & Hay, B. P. (1998, Mar.). A MM3(96) force field for metal-amide complexes. 215th American Chemical Society National Meeting, Dallas, TX.

Hay, B. P. (1998, Aug.). A points-on-a-sphere approach to model metal-ligand interactions with an extended MM3 model. Invited presentation at the 216th American Chemical Society National Meeting, Boston, MA.

Hay, B. P. (1998, Jul.) Architectural design criteria for f-block metal sequestering agents. Environmental Management Science Program Workshop. Chicago, IL.

Hay, B. P. (1998, Oct.). Ligand design with molecular mechanics. INEEL Science Integrated Workshop, Environmental Management Science Program. Idaho Falls, ID.

Hay, B. P. (1999, Jun.) The application of molecular mechanics in the design of metal ion sequestering agents.Invited presentation at the Metal Separation Technologies Beyond 2000: Integrating Novel Chemistry with Processing United Engineering Foundation Conference. Turtle Bay, Oahu, HI.

Hay, B. P., Dixon, D. A., & Sandrone, G. (1998, Jun.). A modified MM3(96) force field for simple amides and diamides. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Hay, B. P., Dixon, D. A., & Sandrone, G. (1998, Jun.). A modified MM3(96) force field for simple amides and diamides. West Coast Theoretical Chemistry Conference. Richland, WA.

Lumetta, G. J., McNamara, B. K., & Burgeson, E. (1997, Jun). Amide complexes of f-block elements. 21st Annual Actinide Separations Conference. Charleston, SC.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1998, Apr.). Binding of amide ligands to f-block elements. 22nd Annual Actinide Separations Conference. Chattanooga, TN.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1998, Jun.). Binding of diamide ligands to f-block elements. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1999, Mar.). Equilibrium modeling of the extraction of f-block elements by diamides. 217th American Chemical Society National Meeting. Anaheim, CA.

Rao, L., Zanonato, P., & Di Bernardo, P. (1998, Aug.). Thermodynamics of europium(III) complexation with alkyl-substituted diamides in organic solvents. 216th American Chemical Society National Meeting. Boston, MA.

Rapko, B. M. (1997, Apr.) Extraction of f-elements by phosphine oxide/pyridine N-oxide ligands. 213th American Chemical Society National Meeting. San Francisco, CA.

Rapko, B. M., et al. (1999, Mar.). Coordination chemistry of tetraalkyldiamides with f-block metal salts. 217th American Chemical Society National Meeting. Anaheim, CA.

Rapko, B. M., et. al. (1999, Jun.). Coordination chemistry of diamides with f-block metal salts. Metal Separation Technologies Beyond 2000: Integrating Novel Chemistry with Processing United Engineering Foundation Conference. Turtle Bay, Oahu, HI.

Rapko, B. M., Lumetta, G. J., McNamara, B. K., Rao, L., & Zanonato, P. L. (1997, Oct.). Determination of actinide and lanthanide binding constants with amides and diamides. Tenth Symposium on Separation Science and Technology for Energy Applications. Gatlinburg, TN.

Rapko, B. M., McNamara, B. K., Rogers, R. D., Lumetta, G. J., & Hay, B. P. (1998, Jun.). Coordination chemistry of lanthanide salts with N,N,N',N'-tetramethylsuccinamide and N,N,N',N'-tetrahexyl-succinamide. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Roundhill, D. M. (1998, May). New macrocycles for selective ion exchange. Metals Adsorption Workshop. Cincinnati, OH.

Roundhill, D. M. (1999, Mar.). Calixarene amines and amides as extractants for oxyions. 217th National American Chemical Society National Meeting. Anaheim, CA.

Yordanov, A. T., Wolf, N. J., Koch, H. F., & Roundhill, D. M. (1998, Jun.). Sulfur and nitrogen derivatized calix[4]arenes as selective phase transfer extractants for heavy metals and oxyions. Second Fargo Conference on Main Group Chemistry. Fargo, ND.

Zanonato, P. L. & Rao, L. (1997, Sept.). Complexation of Eu(III) by N,N,N',N'-tetra-alkyldiamides. 214th American Chemical Society National Meeting. Las Vegas, NV.

Publication Type: Proceeding

Hay, B. P. (1999, in press). The use of molecular mechanics in the design of metal ion sequestering agents. In Metal separation technologies beyond 2000: Integrating novel chemistry with processing. United Engineering Foundation. New York, NY.

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1998). Environmental management science program workshop. CONF-980736, Environmental Management Science Program, U.S. Department of Energy, Office of Science and Risk Policy EM-52. Washington, D.C.

Rao, L., Xia, Y., Rapko, B. M., & Martin, P. L. (1997, Jun). Synergistic extraction of Eu(III) and Am(III) by TTA and the neutral donor extractants CMPO and NOPOPO. 21st Annual Actinide Separations Conference. Charleston, SC.

Publication Type: Report

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1997). Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. Fiscal Year 1997 Mid-Year Progress Report. PNNL-11589, Pacific Northwest National Laboratory. Richland, WA.

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1998). Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. Fiscal Year 1998 Mid-Year Progress Report. PNNL-11899, Pacific Northwest National Laboratory. Richland, WA.

Lumetta, G. J., Rapko, B. M., & McNamara, B. K. (1999). The SX solver: A new computer program for analyzing solvent extraction equilibria. PNNL-12085, Pacific Northwest National Laboratory. Richland, WA.

Project: 54680

Title: The Migration and Entrapment of DNAPLs in Physically and Chemically Heterogeneous Porous Media

PI: Dr. Linda M. Abriola *Institution:* University of Michigan

Publication Type: Journal

Bradford, S. A., Abriola, L. M., & Leij, F. J. (1997). Wettability effects on two- and three- fluid relative permeabilities. Journal of Contam. Hydrol., 28, 171-191.

Bradford, S. A., Abriola, L. M., & Rathfelder, K. M. (1998). Flow and entrapment of dense nonaqueous phase liquids in physically and chemically heterogeneous aquifer formations. Adv. Water Res., 22, 117-132.

Lord, D. L., Hayes, K. F., Demond, A. H., & Salehzadeh, A. (1997). Influence of organic acid solution chemistry on subsurface transport properties. 1. Surface and interfacial tension. Environ. Sci. Technol., 31, 2045-2051.

Lord, D. L., Demond, A. H., Salehzadeh, A., & Hayes, K. F. (1997). Influence of organic acid solution chemistry on subsurface transport properties. 2. Capillary pressure- saturation. Environ. Sci. Technol., 31, 2052-2058.

Publication Type: Other

Lord, D. L. (1999). Influence of organic acid and base solution chemistry on interfacial and transport properties of mixed wastes in the subsurface. Ph.D. dissertation. Department of Civil and Environmental Engineering, The University of Michigan. Ann Arbor, MI.

Publication Type: Paper

Bradford, S. A., & Abriola, L. M. (1998). Entrapment and dissolution of organic liquids in chemically heterogeneous porous media. IAHS Publication no. 250, Groundwater Quality: Remediation and Protection. Tubingen, Germany. 167-172.

Publication Type: Proceeding

Bradford, S. A., Abriola, L. M., & Leij, F. J. (1999, in press). Multi-fluid hydraulic properties for fractional wettability porous media. In Van Genuchten, M. Th., Leij, F. J., & Wu, L. (Eds.), Characterization and Measurement of the Hydraulic Properties for Unsaturated Porous Media, University of California. Riverside, CA.

Bradford, S. A., Abriola, L. M., & Rathfelder, K. M. (1998). Simulated entrapment and dissolution of organic liquids in chemically heterogeneous porous media. In Chrysikopoulos, C. V., Bear, J., & Harmon, T. C. (Eds.), Enviromeet 98- Behavior and Remediation of Nonaqueous Phase Contaminants in the Subsurface. University of California. Irvine, CA. 7-16.

Demond, A.H., Hayes, K. F., Lord, D. L., Desai, F., & Salehzadeh, A. (1999, in press). Impact of organic compound chemistry on capillary pressure relationships of sands. In Van Genuchten, M.Th., Leij, F. J., & Wu, L. (Eds.), Characterization and Measurement of the Hydraulic Properties for Unsaturated Porous Media. University of California. Riverside, CA.

Lord, D. L., Demond, A. H., Hayes, K. F., & Salehzadeh, A. (1999, in press). Effects of surfactant chemistry on interfacial tension, wettability, and capillary pressure in multiphase subsurface waste systems. Transport in Porous Media.

Project: 54683

Title: Speciation and Structural Characterization of Plutonium and Actinide-Organic Complexes in Surface and Groundwaters

PI: Dr. Ken O. Buesseler *Institution:* Woods Hole Oceanographic Institute

Publication Type: Journal

Buesseler, K. O., et. al. (1999, Nov. 16-18). Speciation, mobility, and fate of actinides in the groundwater at the Hanford Site. EMSP PI workshop.

Dai, M., et al. (1999, in press). Size fractionated Pu isotopes in a coastal environment. J. Enivronmental Radioactivity.

Publication Type: Presentation

Dai, M., et al. (1998, May). Size fractionated Pu isotopes in the ocean, a pond and groundwater. AGU Spring Meeting, Boston, MA. EOS, 79(17), 138.

Dai, M., et al. (1999, May). Isotopic composition, speciation and mobility of Pu in the groundwater at DOE Savannah River Site. AGU Spring meeting. Boston, MA.

Dai, M.H., et. al. (1998, July 27- 30). Size fractionated Pu isotopes in surface and subsurface waters. American Chemical Society DOE Environmental Management Science Program Workshop. Chicago, IL.

Repeta, D.J., Quan, T. M., Aluwihare, L. I., & Accardi, A. (1999). Dissolved organic matter in fresh and marine waters. Amer. Soc. Limnol. Oceanogr. Annual meeting. Santa Fe, NM.

Project: 54684

Title: Mechanism Involved in Trichloroethylene-Induced Liver Cancer: Importance to Environmental Cleanup

PI: Dr. Richard J. Bull *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Kato-Weinstein, J., Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1998). Effects of dichloroacetate on carbohydrate metabolism in B6C3F1 mice. Toxicology 130,141-154.

Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1999, in press). Serum insulin levels and differential insulin receptor expression in livers and liver tumors of mice treated with dichloroacetate (DCA). Toxicol. Appl. Pharmacol.

Merdink, J. L., Gonzalez-Leon, A., Bull, R. J., & Schultz, I. R. (1998). The extent of dichloroacetate formation from trichloroethylene, chloral hydrate, trichloroacetate, and trichloroethanol in B6C3F1 mice. Toxicological Sciences 45, 33-41.

Schultz, I. R., Merdink, J. L., Gonzalez-Leon, A., & Bull, R. J. (1999, in press). Comparative toxicokinetics and metabolism of chlorinated and brominated haloacetates in F344 rats. Toxicol. Appl. Pharmacol.

Stauber, A. J., Bull, R. J., & Thrall, B. D. (1998). Dichloroacetate and trichloroacetate promote clonal expansion of anchorage-independent hepatocytes, in vivo and in vitro. Toxicol. Appl. Pharmacol. 150, 287-294.

Publication Type: Poster

Bull, R. J., Minard, K., Sasser, L.B., Lingohr, M. K., & Wind, R.A. (1999). Dichloroacetate-induced liver tumors cease growing on removal of treatment: Result of an insulin-sensitive phenotype? AACR Proceedings 40, 3321

Publication Type: Presentation

Gonzalez-Leon, A., Merdink, J. L., Schultz, I. R., & Bull, R. J. (1998). Dichloroacetate auto-inhibits its degradation in the cytosol. Society of Toxicology, 37th Annual Meeting #426.

Kato-Weinstein, J., Thrall, B. D., & Bull, R. J. (1998). The effect of haloacetates on carbohydrate metabolism in B6C3F1 mice. Society of Toxicology, 37th Annual Meeting #308.

Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1998). Dichloroacetate (DCA) affects proteins involved in insulin signaling in mouse liver cells. Society of Toxicology, 37th Annual Meeting #61.

Merdink, J. L., Schultz, I. R., & Bull, R. J. (1998). Formation of dichloroacetic acid in B6C3F1 mice from trichloroethylene or its metabolites. Society of Toxicology, 37th Annual Meeting #1621.

Mounho, B. J. & Thrall, B. D. (1998). Tumor promotion by peroxisome proliferators may involve the activation of mitogenic activated protein kinases (ERK1/ERK2). Society of Toxicology, 37th Annual Meeting #51.

Orner, G. A., et. al. (1998). Effects of trichloroacetate (TCA) and dichloroacetate (DCA) on H-ras in male B6C3F1 mice. Society of Toxicology, 37th Annual Meeting #60.

Schultz, I. R., Gonzalez-Leon, A., Merdink, J. L., & Bull, R. J. (1998). Comparative toxicokinetics and metabolism of halo-acetic acids in F344 rats. Society of Toxicology, 37th Annual Meeting #1045.

Stauber, A. J., Bull, R. J., & Thrall, B. D. (1998). Dichloroacetate and trichloroacetate promote clonal expansion of anchorage-independent hepatocytes. Society of Toxicology, 37th Annual Meeting #62.

Publication Type: Proceeding

Bull, R. J., Minard, K., Sasser, L. B., Lingohr, M. K., & Wind, R. A. (1999). Dichloroacetate-induced liver tumors cease growing on removal of treatment: Result of an insulin-sensitive phenotype? AACR Proceedings 40, 3321.

Project: 54691

Title: Radiation Effects on Materials in the Near-Field of Nuclear Waste Repository
PI: Dr. Lu-Min Wang *Institution:* University of Michigan

Publication Type: Journal

Gu, B. X., Wang, L. M., & Ewing, R. C. (1999, in press). The effect of amorphization on the Cs ion exchange and retention capacity of zeolite-NaY. Journal of Nuclear Materials.

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999, in press). Electron and ion irradiation of zeolites. Journal of Nuclear Materials.

Publication Type: Proceeding

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999, in press). Electron irradiation of zeolites. Proceedings of the Materials Research Society.

Project: 54716

Title: Polyoxometalates for Radioactive Waste Treatment
PI: Dr. Michael T. Pope *Institution:* Georgetown University

Publication Type: Journal

Dickman, M. H., Gama, G. J., Kim, K. -C., & Pope, M. T. (1996). The structures of europium(III)- and uranium(IV) derivatives of [P 5 W 30 O 110] 15- . Evidence for Cryptohydration. J.Cluster Sci., 7, 67-583.

Kim, K. -C. & Pope, M. T. (1999, in press). Cation-directed structure changes in polyoxometalate chemistry. Equilibria between isomers of bis(9-tungstophosphatodioxouranate(VI)) complexes. J. Am. Chem. Soc.

Müller, A., Peters, F., Pope, M. T., & Gatteschi, D. (1998). Polyoxometalates: Very large structures - nanoscale magnets. Chem. Rev. 98, 239-271.

Pope, M. T., Wei, X., Wassermann, K., & Dickman, M. H. (1998). New developments in the chemistry of heteropolytungstates of rhodium and cerium. C. R. Acad. Sci., 1, Ser. IIc, 297-304.

Wassermann, K., Dickman, M. H., & Pope, M. T. (1997). Self-assembly of supramolecular polyoxometalates. The compact, water-soluble heteropolytungstate anion [As III 12 Ce III 16 (H 2 O)36 W 148 O 524] 76ÿ. Angew. Chem. 109, 1513-1516.

Publication Type: Other

Pope, M. T., Creaser, I. I., & Heckel, M. C. (1997, Apr. 8). Compounds and methods for separation and molecular encapsulation of metalIons. U.S. Patent 5,618,472.

Project: 54724

Title: Synthesis of New Water-Soluble Metal-Binding Polymers: Combinatorial Chemistry Approach
PI: Dr. Barbara F. Smith *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Colletti, L. & Havrilla, G. (1999). Trace element detection with micro-x-ray fluorescence. Advances in X-Ray Analysis, 44.

Kizer, D. E., Miller, R. B., & Kurth, M. J. (1999). Fused pyrazolo heterocycles: intramolecular [3+2]-nitrile oxide cycloadditions applied to syntheses of pyrazolo[3,4-g][2,1]dihydrobenzoisoxazol(in)es. Tetrahedron Letters, 40, 3535-38.

Publication Type: Proceeding

Smith, B. F., Robison, T. W., & Jarvinen, G. D. (1998). Water-soluble metal-binding polymers with ultrafiltration: A technology for the removal, concentration, and recovery of metal ions from aqueous streams. In Rogers, R., Bond, A., & Dietz, M. (Eds.), ACS Symposium Series volume, Advances in Metal Ion Separation and Preconcentration, Chap. 20, 294-330.

Song, J., Corrales, L. R., & Jónsson, H. (1999, in press). Exploring the excited states of vacancy defects in silica. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Project: 54735

Title: Development of Inorganic Ion Exchangers for Nuclear Waste Remediation
PI: Dr. Abraham Clearfield *Institution:* Texas A&M University at College Station

Publication Type: Journal

Khainakov, S. A., et. al. (1999). Hydrothermal synthesis and characterization of alkali metal titanium silicates. Journal of Materials Chem. 9, 269-272.

Pertierra, P., Salvado, M. A., Garcia-Granda, S., Bortun, A. I., & Clearfield, A. (1999). Neutron powder diffraction study of Ti2(OH)2OSiO4.1.5H2O. Inorganic Chem., 38(11), 2563-2566.

Poojary, D. M., Zhang, B., & Clearfield, A. (1998). Synthesis and structures of barium arylbisphosphonates derived from x-ray powder data. Anales de Quimica Int. Ed., 94, 401-405.

Sylvester, P. & Clearfield, A. (1999). The removal of strontium from simulated Hanford tank wastes containing complexants. Separation Science and Technology, 34(13), 2539-2551.

Sylvester, P., Clearfield, A., & Diaz, R. J. (1999). Pillared montmorillonites: cesium-selective ion-exchange materials. Science and Technology, 34(12), 2293-2305.

Trobajo, C., et. al. (1999). Hydrothermal synthesis and ion exchange properties of the novel framework sodium and potassium niobium silicates. Solvent Extraction and Ion Exchange, 17(3), 649-675.

Project: 54741

Title: Characterization of Contaminant Transport Using Naturally-Occurring U-Series Disequilibria

PI: Dr. Michael T. Murrell *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. (1998, Dec. 6-10). Assessing in-situ radionuclide transport based on uranium-series disequilibrium in groundwater. Fall AGU Meeting. San Francisco, CA. EOS Trans. Amer. Geophys. Un. 79, F354.

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. (1999, Aug. 21-26). Uranium-series disequilibria in groundwater: Assessing radionuclide migration. 9th International Conference on Isotope Geology, Cosmochemistry and Geochronology. Beijing, China.

Roback, R. C., et. al. (1997). Groundwater mixing, flow-paths and water/rock interaction at INEEL: Evidence from uranium isotopes. Geological Society of America, Abstracts with Programs, 29(6).

Roback, R. C., et. al. (1998, Dec. 6-10). Uranium and thorium series isotopes in fractured rocks at the INEEL. Fall AGU Meeting. San Francisco, CA. EOS Trans. Amer. Geophys. Un. 79, F343.

Project: 54765

Title: Enhanced Sludge Processing of HLW: Hydrothermal Oxidation of Chromium, Technetium, and Complexants by Nitrate

PI: Dr. Stephen J. Buelow *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Goemans, M. G. E., Funk, T. J., Sedillo, M. A., Buelow, S. J., & Anderson, G. K. (1997). Electrical conductances of aqueous solutions of inorganic nitrates ate 25-505_C and 100-490 bar,î. Journal of Supercritical Fluids 11, 61-72.

Project: 54770

Title: New Anion-Exchange Resins for Improved Separations of Nuclear Materials

PI: Dr. Mary E. Barr *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Marsh, S. F., Jarvinen, G. D., & Bartsch, R. A. (1997). New bifunctional anion-exchange resins for nuclear waste treatment. Reactive Polymers, 35, 75-80.

Marsh, S. F., Jarvinen, G. D., Bartsch, R. A., Nam, J., & Barr, M. E. (1998). New bifunctional anion-exchange resins for nuclear waste treatment-II. J. Radioanal. Nucl. Chem., 235, 37-40.

Publication Type: Presentation

Barr, M. E., Jarvinen, G. D., Marsh, S. F., & Bartsch, R. A. (1997, Apr. 13). Development of anion-exchange resins for separations of actinides. Abstracts of Papers of the American Chemical Society, 213(pt.2), 73-IEC.

Barr, M. E., Jarvinen, G. D., Moody, E. W., & Vaughn, R. B. (1998, Aug. 23). Sorption of Pu(IV) by soluble anion-exchange polymers. Abstracts of Papers of the American Chemical Society, 216(pt.2), 88-NUCL, & 216(pt.1), 5-TECH.

Barr, M. E., Jarvinen, G. D., Schulte, L. D., Stark, P. C., & Chamberlin, R. M. (1999, Mar. 21). Americium separations from complex mixtures using anion exchange. Abstracts of Papers of the American Chemical Society, 217, 019-IEC.

Bartsch, R. A., et. al. (1999, Mar. 21). Sorption of Pu(IV) from nitric acid by bifunctional anion-exchange resins. Abstracts of Papers of the American Chemical Society, 217, 125-IEC.

Marsh, S. F., Jarvinen, G. D., Bartsch, R. A., Nam, J., & Barr, M. E. (1997, Apr.). New bifunctional anion-exchange resins for nuclear waste treatment. Marc IV conference on Radioanalytical Chemistry, Kona, HI.

Moody, E. W., Barr, M. E., & Jarvinen, G. D. (1999). QSAR of distribution coefficients for actinide hexanitrato complexes. Abstracts of Papers of the American Chemical Society, 217(pt.2), 170-NUCL.

Project: 54790

Title: Microbial Mineral Transformations at the Fe(II)/Fe(III) Redox Boundary for Solid Phase Capture of Strontium and Other Metal/Radionuclide Contaminants

PI: Dr. F. Grant Ferris *Institution:* University of Toronto

Publication Type: Journal

Howell, J. R., Donahoe, R. J., Roden, E. E., & Ferris, F. G. (1998). Effects of microbial iron oxide reduction on pH and alkalinity in anaerobic bicarbonate-buffered media: Implications for metal mobility. Mineralogical Magazine, 62A, 657-658.

Publication Type: Other

Howell, J. R. (1998). Effects of microbial Fe(III) oxide reduction on pH, DIC, and carbonate mineral formation: Implications for metal mobility. M. S. Thesis, Department of Geology, University of Alabama. Tuscaloosa, AL.

Publication Type: Presentation

Maurice, P.A., Warren, L. A., & Ferris, F. G. (1998). Calcite precipitation by B. pasteurei: AFM imaging of microbial-mineral interactions. Geological Society of America Annual Meeting. Toronto, Canada.

Parmar, N., Warren, L. A. & Ferris, F. G. (1998). Solid phase capture of strontium by the iron reducing bacteria Shewenella alga. Geological Society of America Annual Meeting. Toronto, Canada.

Small, T.D., Warren, L. A., & Ferris, F. G. (1998). Strontium sorption to bacterial and Fe oxide surfaces. Geological Society of America Annual Meeting. Toronto, Canada.

Warren, L. A., Parmar, N., & Ferris, F. G. (1998). Strontium, uranyl, and copper incorporation in bacterially mediated calcite precipitation. Geological Society of America Annual Meeting. Toronto, Canada.

Publication Type: Proceeding

Warren, L. A. & Ferris, F. G. (1998). Solid phase partitioning of uranium and copper in the presence of HFO and bacteria. In Arehart, G. B. & Hulston, J. R. (Eds.), Proceedings of the 9th International Symposium on Water Rock Interaction WRI-9. Balkema, Rotterdam. 115-117.

Project: 54834

Title: An Investigation of Homogeneous and Heterogeneous Sonochemistry for Destruction of Hazardous Waste
PI: Dr. Inez Hua *Institution:* Purdue University

Publication Type: Presentation

Hua, I. (1999, Feb.). The use of ultrasonic irradiation in environmental engineering processes. Borchardt Conference, The University of Michigan. Ann Arbor, MI.

Pfalzer, U. & Hua, I. (1997, Nov. 9). Sonochemical degradation of carbofuran in a parallel-plate near-field acoustical processor. 20th Annual Midwest Environmental Chemistry Workshop, Indiana University. Bloomington, IN.

Schramm, J. & Hua, I. (1997, Sept.). Degradation of dichlorvos by sonolysis. American Chemical Society Meeting. Las Vegas, NV.

Zhang, G. & Hua, I. (1998, Mar.). Destruction of polychlorinated biphenyls in acoustically cavitating systems. American Chemical Society Meeting. Dallas, TX.

Project: 54837

Title: Phytoremediation of Ionic and Methyl Mercury Pollution
PI: Dr. Richard B. Meagher *Institution:* University of Georgia

Publication Type: Journal

Heaton, A. C. P., Rugh, C. L., Wang, N. -J., & Meagher, R. B. (1998). Phytoremediation of mercury and methylmercury polluted soils using genetically engineered plants. J. Soil Contam. 7, 497-509.

Rugh, C. L., Gragson, G. M., & Meagher, R. B. (1998). Toxic mercury reduction and remediation using transgenic plants with a modified bacterial gene. Hort. Sci. 33, 12-15.

Rugh, C. L., Senecoff, J. F., Meagher, R. B., & Merkle, S. A. (1998). Development of transgenic yellowpoplar for mercury phytoremediation. Nature Biotech. 16, 925-928.

Publication Type: Other

Rugh, C. L., Bizily, S. P., & Meagher, R. B. (1999). Phytoremediation of environmental mercury pollution. In Ensley, B. & Raskin, I. (Eds.), Phytoremediation of toxic metals: Using plants to clean-up the environment. Wiley and Sons, New York, NY.

Publication Type: Paper

Meagher, R. B. & Rugh, C. L. (1996). Phytoremediation of heavy metal pollution: Ionic and methylmercury. OECD Biotechnology for Water Use and Conservation Workshop. Organization for Economic Co-Operation and Development. Cocoyoc, Mexico. 305-321.

Meagher, R. B. (1998). Phytoremediation: An affordable, friendly technology to restore marginal lands in the twenty-first century. Plants and Population: Is there time? Natl. Acad. Sci. Colloquium. Irvine, CA.

Publication Type: Proceeding

Bizily, S., Rugh, C. L., Summers, A. O., & Meagher, R. B. (1999). Phytoremediation of methylmercury pollution: MerB expression in Arabidopsis thaliana confers resistance to organomercurials. Proc. Natl. Acad. Sci. USA 96, 6808-6813.

Meagher, R. B. & Rugh, C. L. (1996). Phytoremediation of heavy metal pollution: Ionic and methylmercury. OECD Biotechnology for Water Use and Conservation Workshop. Organization for Economic Co-Operation and Development. Cocoyoc, Mexico. 305-321.

Meagher, R.B., Rugh, C. L., Kandasamy, M. K., Gragson, G., & Wang, N. J. (1998). Engineered phytoremediation of mercury pollution in soil and water using bacterial genes. In Ishndar, I. K., Hardy, S. E., Chang, A. C., & Pierzynski, G. M. Fourth International Conference on the Biogeochemistry of Trace Elements Ann Arbor Press, Inc. Berkeley, CA. 203-221.

Rugh, C. L., et. al. (1996). Mercuric ion reduction and resistance in transgenic Arabidopsis thaliana plants expressing a modified bacterial merA gene. Proc. Natl. Acad. Sci. USA 93, 3182-3187.

Project: 54847

Title: Photocatalytic and Chemical Oxidation of Organic Compounds in Supercritical Carbon Dioxide

PI: Dr. Daniel M. Blake *Institution:* National Renewable Energy Laboratory

Publication Type: Journal

Jacoby, W. A., et al. (1996). Heterogeneous photocatalysis for control of volatile organic compounds in indoor air. J. Air Waste Manage. Assoc., 46(9), 891-8.

Project: 54864

Title: Supramolecular Chemistry of Selective Anion Recognition for Anions of Environmental Relevance

PI: Dr. Kristin Bowman-James *Institution:* University of Kansas

Publication Type: Journal

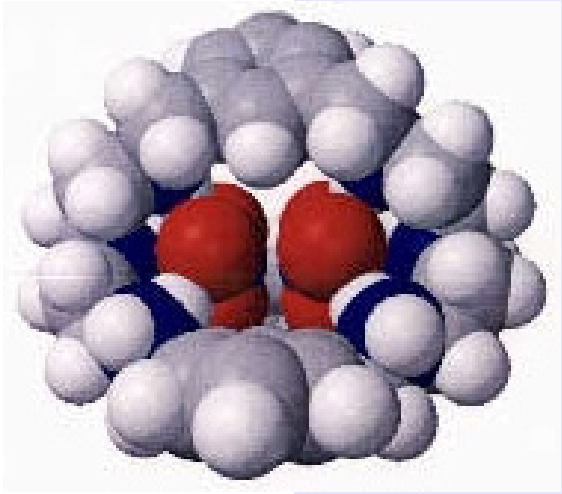
Clifford, T., Mason, S., Llinares, J. M., & Bowman-James, K. (2000). Snap-shots of fluoride binding in an Azacryptand. J. Am. Chem. Soc., 122,1814-1815.

Danby, A., Seib, L., Alcock, N. W., & Bowman-James, K. (1999, in press). Novel structural determination of a bilayer network formed by a tripodal lipophilic amide in the presence of anions. Chem. Commun.

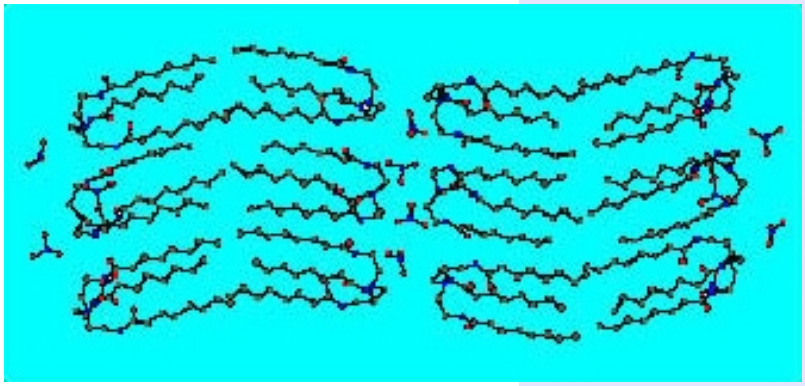
Gerasimchuk, O. A., et. al. (1999, in press). Phosphate binding in a hexaaza polyammonium macrocycle. Inorg. Chem.

Mason, S., Clifford, T., Seib, L., Kuczera, K., & Bowman-James, K. (1998). Unusual encapsulation of two nitrates in a single bicyclic cage. J. Am. Chem. Soc., 120,8899-8900.

Wiórkiewicz-Kuczera, et. al. (1999). Solid state to solution: Crystal structure and molecular dynamics simulations of a polyammonium nitrate host, New J. Chem., 23,1007-1013.



Nitrate inclusion complex with a polyammonium receptor. [see Project #54864]



Contaminant Binding Science - The crystal structure of one of a tripodallipophilic adide with nitrate ion, illustrated above, was developed for a University of Kansas project, which uses a combination of anion and catioin complexing agents to extract cesium nitrate. [see Project #54864]

Publication Type: Press Release

Moyer, B. A. (1998, Sep. 7). Two nitrates in a cage. C&E News concentrate. 30.

Publication Type: Other

Bianchi, A., Bowman-James, K., & García-Espana, E. (Eds.). (1997), Supramolecular Chemistry of Anions, Wiley-VCH. New York, NY.

Wiórkiewicz-Kuczera, J. & Bowman-James, K. (1997). Anion Binding Receptors: Theoretical Studies. In Bianchi, A., Bowman-James, K., & García-España, E. (Eds.), Supramolecular Chemistry of Anions. Wiley-VCH, New York, NY. 335-354.

Project: 54898

Title: Molecular Dissection of the Cellular Mechanisms Involved in Nickel Hyperaccumulation in Plants

PI: Dr. David E. Salt *Institution:* Northern Arizona University

Thlaspi Goesingense growing in its native ultramafic habitat near Redschlag/Austria. The Northern Arizona University team is investigating, at the molecular level, the role of histidine biosynthesis in byperaccumulation in *Thlaspi goesingense*. [see Project #54898]

Publication Type: Journal

Krämer, U., Smith, R. D., Wenzel, W., Raskin, I., & Salt, D. E. (1997). The role of nickel transport and tolerance in nickel hyperaccumulation by Thlaspi goesingense Hálácsy. Plant Physiol, 115, 1641-1650.

Persans, M., Xiange,Y., Patnoe, J. M. M. L., Krämer, U., & Salt, D. E. (1999, in press). Molecular dissection of histidine's role in nickel hyperaccumulation in Thlaspi goesingense (Hálácsy). Plant Physiology.

Persans, M., Yan, X., Smith, R., & Salt, D. E. (1998). Cloning of two cDNA's from the Ni hyperaccumulator Thlaspi goesingense: Histidinol dehydrogenase (Accession No. AF023141) and imidazolglycerol-phosphate dehydratase (Accession No. AF023140), two enzymes in the histidine biosynthetic pathway. Plant Physiol Plant Gene Register, 117, 332.

Salt, D. E., Prince, R. C., Baker, A. J. M., Raskin, I., Pickering, I. J. (1999). Zinc ligands in the metal hyperaccumulator Thlaspi caerulescens as determined using X-ray absorption spectroscopy. Environmental Science and Technology 33, 713-717.

Salt, D. E., Smith, R. D., & Raskin, I. (1998). Phytoremediation. Ann Rev Plant Physiol Plant Mol Biol, 49, 643-668.

Publication Type: Other

Salt, D. E. (1999, in press). Phytoextraction: Present applications and future promise. In Wise, D. L., Trantolo, D. J., Inyang, H. I., & Cichon, E. J. (Eds.), Remediation of Hazardous Waste Contaminated Soils, 2nd Edition, Marcel Dekker, Inc.

Salt, D. E., & Baker, A. J. M. (1999, in press). Phytoremediation of metals. In Rehm, H. -J. & Reed, G. (Eds.),Biotechnology 2nd Edition, Wiley-VCH. New York, NY.

Salt, D. E., & Krämer, U. (1999, in press). Mechanisms of metal hyperaccumulation in plants. In Ensley, B. D. & Raskin, I. (Eds.), Phytoremediation of Toxic Metals: Using Plants to Clean-Up the Environment, Chapter 13, John Wiley & Sons, Inc., New York, NY.

Salt, D. E., Kato, N., Krämer, U., Smith, R. D. & Raskin, I. (1999). The role of root exudates in nickel hyperaccumulation and tolerance in accumulator and non-accumulator species of Thlaspi. In Terry, N. & García-España, X. (Eds.), Phytoremediation of Contaminated Soil and Water, Chapter 10, CRC Press LLC. Boca Raton, FL. 189-200.

Wenzel, W., Salt, D. E., Smith, R. D., & Adriano, D. C. (1999). Phytoremediation: A plant-microbe-based remediation system. In Adriano, D. C., et. al. (Eds.), Bioremediation of Contaminated Soils. American Society of Agronomy Inc., Crop Science Society of America, Inc., Soil Science Society of America, Inc., Madison, Wisconsin. 18, 457-508.

Publication Type: Paper

Special Symposium - Phytoremediation. (1999, Jul. 11-15). Progress towards a molecular understanding of metal hyperaccumulation in plants. 5th International Conference on the Biogeochemistry of Trace Elements. Vienna, Austria.

Publication Type: Presentation

Plenary Address - Phytoremediation as a Clean-Up Technology for the Next Millennium (1999, Jun. 23-25). The Researcher's Perspective - Progress and Bottlenecks. 4th IBC Annual International Conference on Phytoremediation, Toronto, Canada.

Remediation Mini-Symposium. (1999, Jul. 24-28). Towards a molecular understanding of the mechanim of Ni hyperaccumulation in Thlaspi. American Society of Plant Physiologists Annual Meeting. Baltimore, MD.

Project: 54908

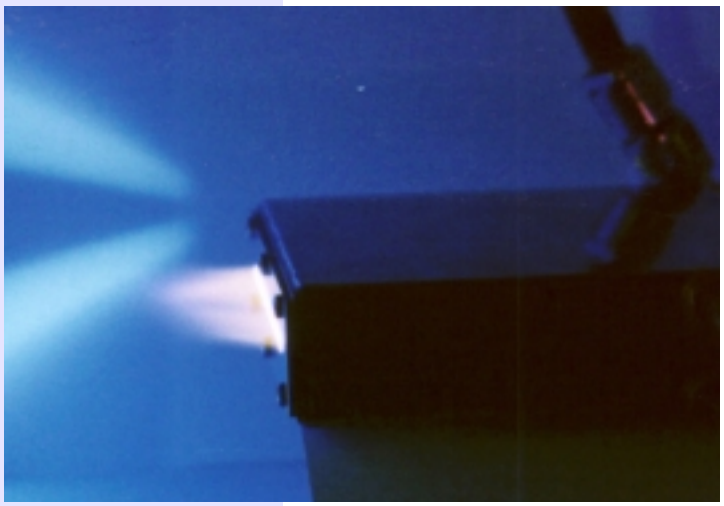
Title: Partitioning Tracers for In Situ Detection and Quantification of Dense Non-aqueous Phase Liquids in Groundwater Systems

PI: Dr. Mark L. Brusseau *Institution:* University of Arizona

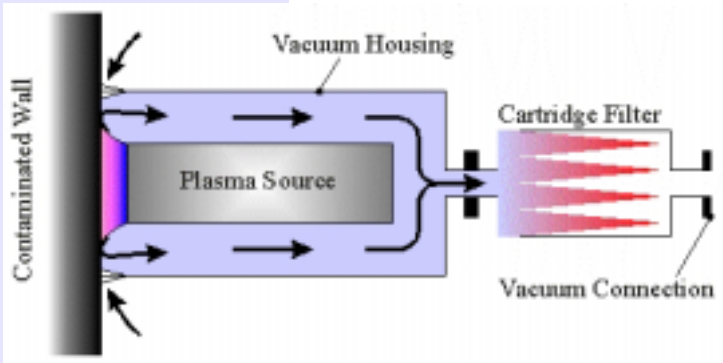
Publication Type: Journal

Brusseau, M. L., Nelson, N. T., & Costanza, M. S. (1999, in press). Partitioning tracer tests for characterizing immiscible-fluid saturations and interfacial areas in subsurface systems.

Nelson, N. T., et. al. (1999, in press). A gas-phase partitioning tracer method for the in-situ measurement of soil-water content. Water Resour. Res.



Side view of a 4" wide atmospheric-pressure plasma source operating with 750 Torr helium and 10 Torr oxygen. [see Project #54914]



Schematic of a method for decontaminating surfaces, such as building wall. The plasma source is mounted within a housing that keeps the pressure slightly below ambient to prevent the etch products from escaping the device. A cartridge filter for the radioactive contaminants can be placed near the plasma source and replaced periodically as needed. [see Project #54914]

Nelson, N. T., Oostrom, M., Wietsma, T. W., & Brusseau, M. L. (1999, in press). The partitioning tracer method for the in-situ measurement of DNAPL saturation: Influence of heterogeneity and sampling method. Environ. Sci. Technol.

Project: 54914

Title: Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces

PI: Dr. Robert F. Hicks

Institution: University of California at Los Angeles

Publication Type: Journal

Babayan, S. E., et. al. (1998, in press). Plasma source science and technology.

Jeong, J. Y., et. al. (1998). Plasma source science and technology, accepted for publication in 1998.

Publication Type: Patent

Selwyn, G. S. (1999, Oct. 5). Atmospheric-pressure plasma jet. US5961772.

Project: 54973

Title: A Novel Energy-Efficient Plasma Chemical Process for the Destruction of Volatile Toxic

PI: Dr. Lal A. Pinnaduwage

Institution: Oak Ridge National Laboratory

Publication Type: Journal

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998). Enhanced negative ion formation by electron attachment to highly-excited molecules in a flowing plasma. J. Appl. Phys. 84,3051.

Ding, W., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999). The role of high Rydberg states in enhanced o-formation in a pulsed O2 discharge. Plasma Sources Sci. Technol. 8,384.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1999). A methodology for direct sampling and gas chromatographic/mass spectral analysis of volatile organic compounds emerging from a low pressure, flow-through reaction cell. J. Chromatography A., 844,217.

Mabel, A. M., Lin, S. H., & Pinnaduwage, L. A. (1998). Potential energy surfaces of H2. Chem. Phys. Lett. 285,114.

McCorkle, D. L., Ding, W. X., Ma, C. Y. & Pinnaduwage, L. A. (1999). Dissociation of benzene in a pulsed glow discharge. J. Appl. Phys. 86,3550.

McCorkle, D. L., Ding, W., Ma, C. Y., & Pinnaduwage, L. A. (1999). Exploratory studies on a plasma remediation process based on enhanced dissociative electron attachment to highly-excited molecules. J. Phys. D., 32,46.

Pinnaduwage, L. A., et. al. (1999). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. J.Appl. Phys., 85,7064.

Pinnaduwage, L. A., McCorkle, D. L., & Ding, W. (1997). Enhanced electron attachment to highly excited molecules using a plasma mixing scheme. Appl. Phys. Lett. 71,3634.

Pinnaduwage, L. A., Tav, C., McCorkle, D. L., & Ding, W. (1999). Temperature dependence of electron attachment to methylene chloride. J. Chem. Phys., 110,9011.

Publication Type: Patent

Pinnaduwage, L. A. (1999, Apr. 20). Plasma mixing glow discharge device for analytical applications. US5896196.

Publication Type: Presentation

Ding, W. X., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Decomposition of volatile organic compounds in a positive column glow discharge plasma. Presentation at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W. X., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999, Mar. 20-26). O- formation by electron attachment to high Rydberg states. Presented at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Ding, W., Ma, C. Y., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Decomposition of volatile organic compounds in a positive column glow discharge plasma. Presented at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Enhanced radical formation by electron attachment to highly-excited states of molecules in plasmas. Presented at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W., McCorkle, D. L., Ma, C. Y., & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociation of benzene in a pulsed glow discharge. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1998, May 31 - Jun. 4). A methodology for direct sampling of volatile organic compounds emerging from a low-pressure, flow-through reaction cell for subsequent GC-GC/MS analysis. Presented at the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando, FL.

McCorkle, D. L. & Pinnaduwage, L. A. (1997, Oct. 6-9). Destruction of CH2Cl2 using a glow discharge scheme. 50th Annual Gaseous Electronics Conference. Madison, WI.

Pinnaduwage, L. A. (1997, Jun. 29 - Jul. 2). Implications of electron attachment to highly-excited states in pulsed power discharges. 11th IEEE Pulsed Power Conference. Baltimore, MA.

Pinnaduwage, L. A. (1999, Sep. 22). Novel energy-efficient plasma chemical process for the destruction of volatile toxic compounds. DOE Environmental Management Science Program Workshop. Oak Ridge, TN.

Pinnaduwage, L. A., Datskos, P. G., Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to highly-excited states of molecules: Implications for plasma processing discharges. Presentation at the 1998 International Congress on Plasma Physics. Prague, Czech Republic.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Presented at the 1998 International Congress on Plasma Physics. Prague, Czech Republic.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999, Mar. 20-26). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. Presented at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999, Jun. 27-30). Implications of electron attachment to highly-excited states of molecules and its applications in pulsed plasmas. 12th IEEE Pulsed Power Conference. Monterrey, CA.

Pinnaduwage, L. A., Ding, W., & McCorkle, D. L. (1999, Oct. 5-8). Negative ion formation in pulsed plasmas. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Pinnaduwage, L. A., Ma, C. Y., McCorkle, D. L., & Ding, W. (1998, Jul. 27-30). A novel energy-efficient plasma chemical process for the destruction of volatile toxic compounds. Presented at the Environmental Management Science Program Workshop. Chicago, IL.

Tav, C. & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociative electron attachment to laser-excited benzene. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Publication Type: Proceeding

Pinnaduwage, L. A. (1997). Implications of electron attachment to highly-excited states in pulsed power discharges. In Cooperstein, G. & Vitkovitsky, I. (Eds.), Digest of Technical Papers of the 11th IEEE Pulsed Power Conference. IEEE Publishing Services. New York, NY. 1048-1053.

Pinnaduwage, L. A., Datskos, P. G., Ding, W. X., & McCorkle, D. L. (1999). Enhanced electron attachment to highly-excited states of molecules: Implications for plasma processing discharges. Pavlo, P. (Ed.). Proceedings of the 1998 International Congress on Plasma Physics. 125-128.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Pavlo, P. (Ed.). Proceedings of the 1998 International Congress on Plasma Physics. 129-132.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999, in press). Enhanced electron attachment to highly-excited molecules and its applications in pulsed plasmas. Digest of Technical Papers of the 12th IEEE Pulsed Power Conference. IEEE Publishing Services. New York, NY.

Project: 54996

Title: Ionizing Radiation Induced Catalysis on Metal Oxide Particles
PI: Dr. Michael A. Henderson *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Epling, W. S., Peden, C. H. F., Henderson, M. A., & Diebold, U. (1998). Evidence for oxygen adatoms on TiO2(110) resulting from O2 dissociation at vacancy sites. Surf. Sci. 412-413, 333.

Henderson, M. A., Epling, W. S., Perkins, C. L., Peden, C. H. F., & Diebold, U. (1999, in press). Interaction of molecular oxygen with the vacuum annealed TiO2(110) surface: Molecular and dissociative channels. J. Phys. Chem.

Henderson, M. A., Oreto-Tapia, S., & Castro, M. E. (1998). Electron induced decomposition of CH3OH on the vacuum annealed surface of TiO2(110). Surf. Sci. 412-413, 252.

Herman, G. S., Henderson, M A., Starkweather, K. A., & McDaniel, E. P. (1999, in press). Mass- spectrometry of recoiled ions and secondary ion mass spectrometry investigation of Y-stabilized ZrO2(100) and (110). J. Vac. Sci. Technol. A.

Su, Y., et. al. (1998). Gamma-ray destruction of EDTA catalyzed by titania. J. Adv. Oxid. Technol. 3, 63.

Taylor, D. P., Simpson, W. C., Knutsen, K., Henderson, M. A., & Orlando, T. M. (1998). Photon stimulated desorption of cations from yttria-stabilized cubic ZrO2(100). Appl. Surf. Sci. 102, 4536.

Publication Type: Presentation

Henderson, M. A. (1998). Coadsorption studies with water and oxygen: A small step toward understanding the surface chemical and photochemical properties of TiO2. Invited presentation at the Department of Chemistry, University of Puerto Rico. Mayaquez, Puerto Rico.

Henderson, M. A. (1998). Coadsorption studies with water: A small step toward understanding the surface chemical and photochemical properties of TiO2. Invited presentation at the 45th National Symposium of the American Vacuum Society. Baltimore, MA.

Henderson, M. A. (1998). Ionizing radiation induced catalysis: Radiocatalytic degradation of organic contaminants in TiO2 suspensions. Invited presentation at the Notre Dame Radiation Laboratory, University of Notre Dame. South Bend, IN.

Henderson, M. A. (1999). Activation of molecular oxygen on TiO2(110) by reaction with bridging hydroxyls. First International Workshop on Oxide Surfaces. Elmau, Germany.

Su, Y. (1999, May 24-28). Radiocatalytic and photocatalytic studies of metal ion reduction and water cleavage into hydrogen. The 5th International Conference on Advanced Oxidation Technologies for Water and Air Remediation, Albuquerque, NM.

Su, Y. (1999, May 2-6). Radiocatalytic and photocatalytic studies of oxidation of organics and reduction of water. The 195th Meeting of the Electrochemical Society, Seattle, WA.

Project: 55011

Title: Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes

PI: Dr. James G. Berryman *Institution:* Lawrence Livermore National Laboratory

Publication Type: Journal

Borcea, L., Berryman, J. G., & Papanicolaou, G. C. (1999). Matching pursuit for imaging high contrast conductive media. Inverse Problems, Vol. 15, 811—849.

Dorn, O., Bertete-Aguirre, H., Berryman, J. G., & Papanicolaou, G. C. (1999, in press). A nonlinear inversion method for 3D-electromagnetic imaging using adjoint fields. Inverse Problems.

Publication Type: Paper

Berge, P. A. & Berryman, J. G. (1999, Mar. 24-27). Developing rock physics algorithms for velocity-porosity relations with environmental geophysics applications. Invited presentation at the Fifth SIAM Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX.

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1999, Mar. 14-18). Comparing geophysical measurements to theoretical estimates for soil mixtures at low pressures. Invited presentation in the 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. 465—472.

Buettner, H. M. & Berryman, J. G. (1999, Mar. 14-18). An electromagnetic induction tomography field experiment at Lost Hills, CA. Invited presentation at the 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP), Oakland, CA. 663—672.

Champagne II, N. J., Berryman, J. G., Buettner, H. M., Grant, J. B. & Sharpe, R. M. (1999, Mar. 14-18). A finite-difference frequency-domain code for electromagnetic induction tomography. Poster and paper in 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP), Oakland, CA. 931—940.

Publication Type: Patent

Berryman, J. G. (1998, Dec. 8). Robust discrimination of porosity and fluid saturation using seismic velocity analysis. Patent disclosure IL-10437.

Berryman, J. G. (1998, Nov. 6). Joint inversion of electrical and electromagnetic tomography data for mapping saturation level and connectivity of conducting fluids underground. Patent disclosure IL-10412.

Publication Type: Presentation

Berryman, J. G. (1997, Aug. 25-29). Challenges for computational physics in underground imaging of electrically conducting contaminant plumes. Invited presentation P2.03 in special session on Geological Phenomena at the International Conference on Computational Physics. American Physical Society, Division of Computational Physics. Santa Cruz, CA.

Berryman, J. G. (1998, Oct. 19-23). Underground imaging of electrically conducting plumes. Invited presentation at the International Advanced Studies Institute, First International Symposium on Detection and Analysis of Subsurface Objects and Phenomena, Naval Postgraduate School. Monterey, CA.

Berryman, J. G., Berge, P. A. & Bonner, B. P. (1999, Nov. 4). Role of lambda-diagrams in estimating porosity and saturation from seismic velocities. Invited presentation at SEG, Houston, TX.

Publication Type: Proceeding

Berge, P. A., Roberts, J. J., Berryman, J. G., & Wildenschild, D. (1998, Jul. 27-30). Joint inversion of geophysical data for site characterization and restoration monitoring. Abstract #188 in Proceedings of Environmental Sciences Management Workshop. Chicago, IL. 378—380.

Berryman, J. G. (1998, Jul. 27-30). Surface and borehole electromagnetic imaging of conducting contaminant plumes. Abstract #189 in Proceedings of Environmental Sciences Management Workshop. Chicago, IL. 380-382.

Berryman, J. G., Champagne II, N. J., & Buettner, H. M. (1999, Oct. 27-29). A 3D finite-difference frequency-domain code for electromagnetic induction tomography. Proceedings of the Second International Symposium on Three Dimensional Electromagnetics, University of Utah. Salt Lake City, UT.

Project: 55013

Title: Biofiltration of Volatile Pollutants: Engineering Mechanisms for Improved Design, Long-term Operation, Prediction and Implementation

PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Barton, J. W., Davison, B. H., Klasson, K. T., & Gable III, C. C. (1999). Estimation of mass transfer and kinetics in operating trickle-bed bioreactors for removal of VOCs. Environ. Prog. 18,87-92.

Barton, J. W., Hartz, S., Klasson, K. T., & Davison, B. H. (1997). Microbial removal of alkanes from dilute gaseous waste streams: Mathematical modeling of advanced bioreactor systems. J. Chem. Technol. Biotechnol.72,93-98.

Barton, J. W., Klasson, K. T., & Davison, B. H. (1997). Microbial removal of alkanes from dilute gaseous waste streams: Kinetics and mass transfer considerations. Biotechnology Progress, 13,814-821.

Davison, B. H., Barton, J. W., Klasson, K. T., & Franciso, A. B. (1999, in press). The influence of high biomass concentrations on alkane solubities. Biotechnology and Bioengineering.

Francisco, A. F., Barton, J. W., Klasson, K. T., & Davison, B. H. (1999, in press). Nutrient limitation effects on a microbial consortium in trickle-bed bioreactors.

Klasson, K. T., Barton, J. W., & Davison, B. H. (1999, Jun.). Performance of a propane-degrading bacterium. Proceedings of the 92nd annual meeting of the Air and Waste Management Association. St. Louis, MO.

Publication Type: Presentation

Barton, J. W. (1998, Jul.). Fundamental mechanisms for improved design, long-term operation, prediction, andimplementation. EMSP Review Meeting. Chicago, IL.

Barton, J. W., Davison, B. H., Klasson, K. T., Gable, III, C. C. (1997, Nov.). Estimation of mass transfer and kinetics in operating biofilters for removal of VOC's. AICHE Annual Meeting. Los Angeles, CA.

Barton, J. W., Klasson, K, T., & Davison, B. H. (1997, Aug. 6-8). Extended performance and evaluation of trickle bed bioreactors designed for VOC removal. Southern Section Annual Meeting of the Air & Waste Management Association. Gaitlinburg, TN.

Barton, J. W., Klasson, K. T., & Davison, B. H. (1997). Extended operation and control of biomass overgrowth in biofilters designed for VOC removal. Presented at the 90th Annual Meeting & Exhibition of Air & Waste Management Association. Toronto, Ontario, Canada.

Barton, J. W., Zhang, X. S., Klasson, K. T., & Davison, B. H. (1998). Predictive mathematical modeling of trickling bed biofilters for elucidating mass transfer and kinetic effects. Presented at the Air & Waste Management Association's 91st Annual Meeting & Exhibition. San Diego, CA.

Davison, B. H. (1999, Mar. 23). Effect of biomass on the measured solubility of sparingly soluble organics in aqueous bioremediation systems. The 217th American Chemical Society Meeting. Anaheim, CA.

Klasson, K. T., Barton, J. W., & Davison, B. H. (1999, Jun.). Performance of a propane-degrading bacterium. 92nd Annual Meeting of the Air and Waste Management Association. St. Louis, MO.

Klasson, K. T., Davison, B. H., Barton, J. W., Just, E. M., & Gable, II, C. C. (1997, Sep.). Biofiltration of chlorinated and non-chlorinated alkanes. Platform presentation at the American Chemical Society's Emerging Technologies in Hazardous Waste Management IX (Enviro Expo '97). Pittsburgh, PA.

Publication Type: Proceeding

Barton, J. W., Zhang, X. S., Klasson, K. T., & Davison, B. H. (1999, Oct. 22-23). Predictive mathematical modeling of trickling bed biofilters. Proceedings of the 1998 USC-TRG Conference on Biofiltration. Los Angeles, CA.

Barton, J. W., Zhang, X. S., Klasson, K. T., & Davison, B. H. (1998, Jun.). Predictive mathematical modeling of trickling bed biofilters for elucidating mass transfer and kinetic effects. Proceedings of the 91st Annual Meeting of the Air & Waste Management Association. San Diego, CA. Paper 98-WAA.13P.

Klasson, K. T., Davison, B. H., Barton, J W., & Jacobs, J. E. (1998, Jun.). Removal of chlorinated and nonchlorinated alkanes in a trickling bed biofilter. Proceedings of the 91st Annual Meeting of the Air and Waste Management Association. San Diego, CA. Paper 98-WAA.06P.

Klasson, K. T., Davison, B. H., Barton, J. W., & Jacobs, J. E. (1998). Removal of chlorinated and non-chlorinated alkanes in a trickle-bed reactor. Proceedings of the 91st Annual Meeting of the Air & Waste Management Association. San Diego, CA.

Publication Type: Theses/Dissertations

DeLozier, G. C. (1998, Dec.). Isolation and identification of VOC metaolizing microorganisms from an active biotrickling filter. Master's Thesis, School of Biotechnology, University of Tennessee. Knoxville, TN.

Project: 55014

Title: Kinetics and Mechanisms of Metal Retention/Release in Geochemical Processes in Soil

PI: Dr. Robert W. Taylor *Institution:* Alabama A&M University

Publication Type: Journal

Shen, S., Taylor, R. W., Bart, H., & Tu, S. (1999, in press). Equilibrium and spectroscopic studies of lead retention in smectite. Commun. Soil Sci. Plant Analysis.

Publication Type: Presentation

Bleam, W. F., et. al. (1998). Recent advances in understanding the chemistry of Cr(VI), Pb(II) and Hg(II) in soils. Agronomy Abstracts. Baltimore, MD. 36.

Shen, S., Taylor, R. W., Bleam, W. F., & Tu, S. I. (1998). Coupled reduction-sorption of chromate in dithionite-reduced smectites. Agronomy Abstracts. Baltimore, MD. 189.

Szulczewski, M. D., Xia, K., Helmke, P. A., Bleam, W. F., & Taylor, R. W. (1998). Evaluating the reductive capacity of humic substances: Reactions between thiol/thio groups and chromate. Agronomy Abstracts, Baltimore, MD. 38.

Taylor, R. W., Shen, S., Bleam, W. F., & Tu, S. (1999, Jul. 11-15). Chromate removal by dithionite-reduced clays. 5th International Conference on the Biogeochemistry of Trace Elements. Vienna, Austria.

Project: 55031

Title: Genetic Analysis of Stress Responses in Soil Bacteria for Enhanced Bioremediation of Mixed Contaminants

PI: Dr. Kwong-Kwok Wong *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Markillie, L. M., Varnum, S., Hradecky, P., & Wong, K. K. (1999). Targeted mutagenesis by duplication insertion in the radioresistant bacterium Deinococcus radiodrans: Radiation sensitivities of catalase (katA) and superoxide dismutase (sodA) mutants. Journal of Bacteriology, 181, 666-669.

Project: 55033

Title: Characterization of Chemically Modified Hyperthermophilic Enzymes for Chemical Syntheses and Bioremediation Reactions

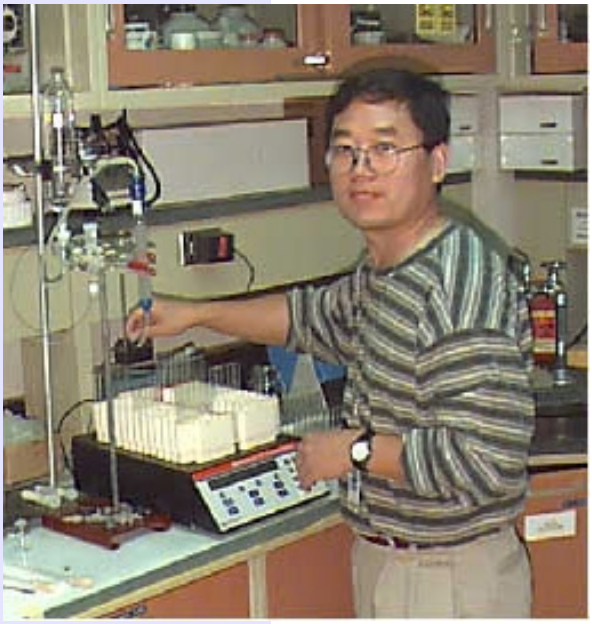
PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Kim., C., Woodward, C. A., Kaufman, E. N., & Adams, M. W. W. (1999). Stability and sulfur reduction activity in organic media of hydrogenase from the hyperthermophilic Pyrococcus furiousus. Biotechnologies & Bioengineering. 65,108-113.

Telser, J., Davydov, R., Kim, C-H., Adams, M. W. W., & Hoffman, B. M. (1999). Investigation of the unusual electronic structure of Pyrococcus furiosis 4Fe ferredoxin by EPR spectroscopy of protein reduced at ambient and cryogenic temperatures. Inorganic Chemistry. 38,3550-3553.

Wang, P., Woodward, C. A., & Kaufman, E. N. (1999). Poly(ethylene glycol)-modified ligninase enhances pentachlorophenol biodegradation in water-solvent mixtures. Biotechnologies & Bioengineering. 64,290-297.



Purification of the PEG-modified enzymes using gel permeation chromatography. [see Project #55033]

Publication Type: Poster

Adams, M. W. W. (1995). Properties of polyethylene glycol-modified proteins in aqueous and organic media. Inorganic Biochemistry Summer Workshop '95. Athens, GA.

Adams, M. W. W. (1996). Polyethylene glycol-modified hydrogenase from pyrococcus furiosis that is soluble and active in organic solvents. Thermophiles '96: International Conference on the Biology, Ecology, and Biotechnology of Thermophilic Microorganisms. Athens, GA.

Wang, P., et. al. (1998, May). PEG-modified ligninase enhances pentachlorophenol biodegradation in water-solvent mixtures. NSF Thermophile Workshop. Seattle, WA.

Publication Type: Presentation

Adams, M. W. W. (1996). Enzymatic catalysis in organic solvents: Polyethylene glycol modified hydrogenase is soluble in toluene and retains sulfur-reducing activity. The 18th Symposium on Biotechnology for Fuels and Chemicals. Gatlingburg, TN.

Adams, M. W. W. (1998, Jul.). Characterization of chemically modified enzymes for bioremediation reactions. EMSP Review Meeting. Chicago, IL.

Davison, B. (1998, May). A new phase for nonaqueous biocatalysis. Oak Ridge National Laboratory Showcase Seminar.

Kaufman, E., et. al. (1996, Nov.). Enzymatic catalysis in organic solvent: Polyethylene glycol modified hydrogenase retains sulfohydrogenase activity in tolunene. AIChE Annual Meeting.

Wang, P., et. al. (1998, May). Modification of enzymes for non-aqueous catalysis: Bioremediation of chlorinated pollutants in organic solvents. 1st Annual Conference on the Remediation of Chlorinated and Recalcitrant Compounds. Columbus, OH.

Wang, P., et. al. (1998, Nov.). Activation and stabilization of ligninase for remediation of polychlorinated pollutants in organic solvents. AIChE Annual Meeting. Miami Beach, FL.

Publication Type: Proceeding

Adams, M. W. W. (1996). Hyperthermophilic proteins from Pyrococcus furiosis that are soluble and active in a pure organic solvent. The 3rd Annual National Science Foundation Hyperthermophile Symposium. Raleigh, NC.

Adams, M. W. W. (1997). Enzymatic catalysis in organic solvents. The 4th Annual National Science Foundation Hyperthermophile Symposium. Del Mar, CA.

Adams, M. W. W. (1998). Catalytic and spectroscopic studies of polyethylene glycol-modified, hyperthermophilic proteins in organic solvents. The 5th Annual National Science Foundation Hyperthermophile Symposium. Seattle, WA.

Adams, M. W. W. (1999). Properties of the ferredoxin iron-sulfur cluster from the hyperthermophilic archaeon Pyrococcus furiosis in organic solvents. The 6th Annual National Science Foundation Hyperthermophile Symposium. Athens, GA.

Project: 55036

Title: Colloid Transport and Retention in Fractured Deposits
PI: Dr. John F. McCarthy *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

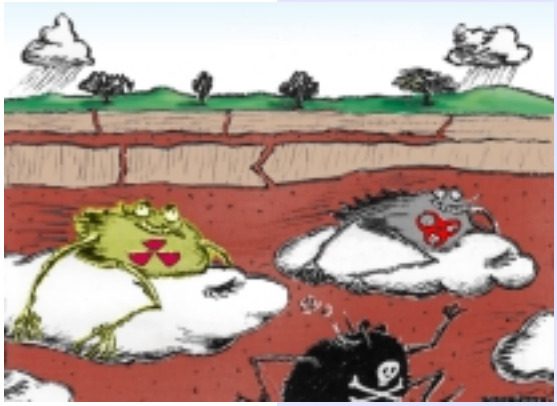
Cumbie, D. H. & McKay, L. D. (1999). Influence of diameter on particle transport in a fractured shale saprolite. J. Contam. Hydrol., 37,139-157.

McCarthy, J. F. & Shevenell, L. (1998). Obtaining representative ground water samples in fractured and karst formations. Ground Water, 36(2),251-260.

McCarthy, J. F. & Shevenell, L. (1998). Processes controlling colloid composition in a fractured and karstic aquifer in eastern Tennessee, USA. J. Hydrol., 206(3-4),191-218.

McCarthy, J. F., Howard, K. M., & McKay, L. D. (1999, in press). Effect of pH on transport of flourobenzoic acid groundwater tracers. J. Contam. Hydrol.

McCarthy, J. F., Howard, K. M., & McKay, L. D. (2000, in press). Influence of pH on the behavior of fluorobenzoic acids as groundwater tracers. J. Environ. Qual.



Mobile colloids in the subsurface environment may alter the transport of contaminants. [see Project #55036]

Publication Type: Theses/Dissertations

Cumbie, D. (1997). Laboratory scale investigations into the influence of particle diameter on colloid transport in a highly fractured shale saprolite. Masters thesis at the University of Tennessee.

Cumbie, D. H. (1997). Influence of diameter on particle transport in a fractured shale saprolite. Master's Thesis. University of Tennessee. Knoxville, TN.

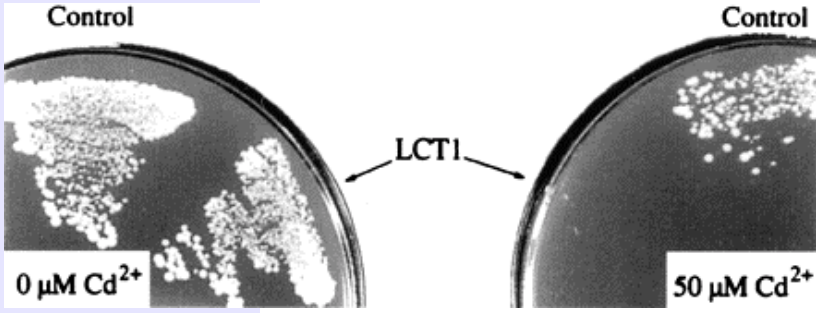
Haun, D. D. B. (1998). Influence of ionic strength and cation valence on transport of colloid-sized microspheres in fractured shale saprolite. Master's Thesis. University of Tennessee. Knoxville, TN.

Howard, K. H. (1997). Behavior of flourobenzoic acid groundwater tracers in a highly fractured shale saprolite. Masters thesis at the University of Tennessee.

Howard, K. H. (1998). Influence of pH on the behavior of fluorobenzoic acids as groundwater tracers. Master's Thesis. University of Tennessee. Knoxville, TN.

Oswald, J. (1999). Numerical modeling of colloid transport in discretely fractured porous media. PhD dissertation at Ohio State University.

Oswald, J. (projected 2000). Migration of colloids in discretely-fractured porous media: Effect of matrix diffusion. Ph. D. dissertation. Ohio State University. Columbus, OH.



LCT1 Mediates Cadmium Uptake. Expression of the wheat gene, LCT1, in *S. cerevisiae* leads to dramatic hypersensitivity to cadmium, and increased intracellular accumulation.
Clemens, S. *et. al* . (1998) *Proc. Natl. Acad. Sci. USA* **95**, 12043-12048. [see Project #55041]

Project: 55041

Title: Molecular Characterization of a Novel Heavy Metal Uptake Transporter from Higher Plants & Its Potential for Use in Phytoremediation
PI: Dr. Julian I. Schroeder
Institution: University of California at San Diego

Publication Type: Journal

Clemens, S., Kim, E. J., Neumann, D., & Schroeder, J. I. (1999). Tolerance to toxic metals by a gene family of phytochelatin synthases from plants and yeast. EMBO J. 18, 3325-3333.

Project: 55052

Title: Advanced Sensing and Control Techniques to Facilitate Semi-Autonomous Decommissioning
PI: Dr. Robert J. Schalkoff *Institution:* Clemson University

Publication Type: Journal

Costescu, N., Loffler, M., Zergeroglu, E., & Dawson, D. (1998, in press). Q robot - a multitasking PC based robot control system. Microcomputer Applications Journal Special Issue on Robotics.

Geist, R., Schalkoff, R., Stinson, T., & Gurbuz, S., (1997). Autonomous virtualization of real environments for telepresence applications. PRESENCE: Teleoperators and Virtual Environments, 6,6. MIT Press, 645 -657.

Publication Type: Proceeding

Costescu, N., Loffler, M., Zergeroglu, E., & Dawson, D. (1998, Sept.). Q robot: A Multitasking PC based robot control system. Proceedings of the IEEE Conference on Control Applications. Trieste, Italy. 892-896.

Geist, R., Vernon, D., & Schalkoff, R. (1998, Apr.). Rendering inversion in the automated construction of virtual environments. Proceedings of the 3rd ASCE Specialty Conf. on Robotics for Challenging Environments (ROBOTICS '98). Albuquerque, NM. 85 - 91.

Geist, R., Westall, J., Tregila, D., & Smotherman, M. (1998, Dec.). Real-time, 3-D graphics for the Linux PC. Proceeds of the 24th Annual Int. Conf. of the Computer Measurement Group (CMG98), Anaheim, CA. 863 - 873.

Van Pernis, A. (1999, Apr.). Surface construction from within a virtual environment. Proceedings of the Annual ACM Southeast Conference. Mobile, AL. NOTE: this was the winning paper in the ACM SE student paper competition.

Project: 55083

Title: Behavior of Dense, Immiscible Solvents in Fractured Clay-Rich Soils
PI: Dr. Larry D. McKay *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

O-Hara, S. K., Parker, B. L., Jorgensen, P. R., & Cherry, J. A. (1999, in press). Trichloroethene DNAPL flow and mass distribution in naturally fractured clay. 1) Evidence of aperture variability. Water Resources Research.

Publication Type: Other

O'Hara, S. K. (1997). Solvent DNAPL flow and matrix diffusion in natural fractured clay: A large column experiment. MS thesis, Univ. of Waterloo. Ontario, Canada.

Publication Type: Paper

Cropper, S.C. (1998). Experimental observations of capillary pressure - saturation drainage of air and DNAPL in fractured shale saprolite. MS Thesis, Univ. of Tennessee. Knoxville, TN.

Publication Type: Presentation

Lenczewski, M., McKay, L. D., Sanseverino, J., & Knight, C. (1998, May 14-16). Sorption and microbiological factors controlling the fate and transport of TCE in fractured shale saprolite. Conference on Mass Transport in Fractured Aquifers and Aquitards, Univ. of Copenhagen, Denmark.

Lenczewski, M., McKay, L. D., Sanseverino, J., & Layton, A. (1999, May 30 - Jun. 3). Biodegradation of TCE in fractured weathered shale in east Tennessee. Annual Meeting of the American Society of Microbiology. Chicago, IL.

Lenczewski, M., McKay, L. D., Sanseverino, J., & Layton, A. (1999, Apr. 12-14). Biodegradation of TCE in fractured shale saprolite. Annual Meeting of the Tennessee Water Resources Association. Nashville, TN.

McKay, L., et al., (1998, Jul. 27-30). Behavior of dense, immiscible solvents in fractured clay-rich soils. Poster presented at DOE/EMSP Workshop. Chicago, IL.

McKay, L.D. (1998, May 14-16). Contaminant transport in highly weathered and fractured shales. Conference on Mass Transport in Fractured Aquifers and Aquitards. Univ. of Copenhagen, Denmark.

McKay, L.D. (1999, May 11-13). Field and laboratory studies of DNAPL behavior in fractured and highly weathered shale. University Consortium Solvents-in-Groundwater Workshop, Queen's University. Kingston, Ontario, Canada.

O'Hara, S. (1999, May 11-13). Characterizing solvent DNAPL migration pathways in fractured clay using a large column laboratory experiment. University Consortium Solvents-in-Groundwater Workshop, Queen's University. Kingston, Ontario, Canada.

O'Hara, S. K., Parker, B. L., Slough, K. J., & Sudicky, E. A. (1998, Dec.). Characterizing solvent DNAPL migration pathways in fractured clay using a numerical model and a large column laboratory experiment. American Geophysical Union (AGU) Fall Meeting, San Francisco, CA.

Parker, B. L., O'Hara, S. K., & Kirkpatrick, G. A. (1998, May 18-21). Solvent DNAPL flow in naturally fractured clay: Laboratory and field experiments. Presented at the First International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA.

Parker, B.L. (1998, May 14-16). Diffusion profiles for identifying DNAPL migration pathways in a glaciolacustrine fractured clay. Conference on Mass Transport in Fractured Aquifers and Aquitards. Univ. of Copenhagen, Denmark.

Pitner, A., McKay, L. D., & Lenczewski, M. (1999, Apr. 12-14). DNAPL entry, dissolution, and diffusion in fractured shale saprolite. Annual Meeting of the Tennessee Water Resources Association. Nashville, TN.

Project: 55087

Title: Design and Synthesis of the Next Generation of Crown Ethers for Waste Separations: An Inter-Laboratory Comprehensive Proposal

PI: Dr. Bruce A. Moyer *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Bond, A. H., et. al. (1999). Synergistic solvent extraction of alkaline Earth cations by mixtures of Di-n-octylphosphoric acid and stereoisomers of Dicyclohexano-18-crown-6. Anal. Chem., 71,2757-2765.

Project: 55094

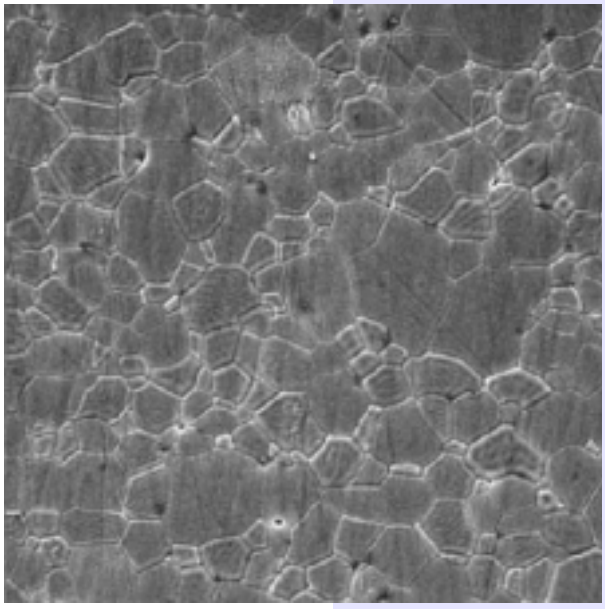
Title: Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite

PI: Dr. P. E. D. Morgan *Institution:* Rockwell International Corporation

Publication Type: Journal

Devanathan, R., Weber, W. J., & Boatner, L. A. (1998). Response of zircon to electron and Ne+ irradiation. Ma, E., Bellon, P., Atmon, M., & Trivedi, R. (Eds.). Phase Transformation and Systems Driven far from Equilibrium. Materials Research Symposium Proceedings, 481,419-424. Boston, MA.

Liu, G. K., Beitz, J. V., Huang, J., Abraham, M. M., & Boatner, L. A. (1997). Characterization of crystal field and nuclear quadrupole interactions in the 5D1 state of 243Am3+ in LaCl3 and CaWO4. Journal of Alloys and Compounds, 250,347-351.



Fully Dense, Stoichiometric La-Monazite, $LaPO_4$, ceramic, sintered to 1400?C - grain size ~2ìm. [see Project #55094]

Liu, G. K., et. al. (1998). Crystal-field splitting, magnetic interaction, and vibronic excitations of 244Cm3+ in YPO4 and LuPO4. Journal of Chemical Phys., 109,6800-6808.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1997). Displacive radiation effects in the monazite- and zircon-structure orthophosphates. Phys. Rev. B, 56,13805.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1997). Electron-irradiation-induced nucleation and growth in amorphous LaPO4 and ScPO4, and zircon. Journal of Materials Research, 12,1816.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1997). Electron-irradiation-induced crystallization of amorphous orthophosphates. Diaz de la Rubia, T., Was, G. S., Robertson, I. M., & Hobbs, L. W. (Eds.). Microstructure Evolution During Irradiation. Materials Research Society Symposium Proceedings, 439,697-702.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1998). Effects of ionizing and displacive irradiation on several perovskite-structure oxides. Nuclear Instrum. Methods Phys. Res. B, 141,347-352.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1998). Phase transitions during ion-beam irradiation of the Perovskite-structure oxides. Ma, E., Bellon, P., Atmon, M., & Trivedi, R. (Eds.). Phase Transformation and Systems Driven far from Equilibrium. Materials Research Symposium Proceedings, 481,401-406. Boston, MA.

Meldrum, A., Boatner, L. A., & Zinkle, S. J. (1999). Effects of dose rate and temperature on the crystalline-to-metamict transformation in the ABO sub-4 Orthosilicates. Canadian Mineralogist, 37,207-221.

Meldrum, A., Boatner, L. A., Wang, L. M., & Ewing, R. C. (1997). Ion-beam-induced amorphization of LaPO4 and ScPO4. Nuclear Instrum. Methods Phys. Res. B, 127/128,160.

Meldrum, A., Boatner, L. A., Weber, W. J., & Ewing, R. C. (1998). Radiation damage in zircon and monazite. Geochim. Cosmochim. Acta, 62,2509-2520.

Meldrum, A., Zinkle, S. J., Boatner, L. A., & Ewing, R. C. (1998). A transient liquid-like phase in the displacement cascades of zircon, hafnon, and thorite. Nature, 395,56-58.

Nipko, J. C., et. al. (1997). Lattice dynamics of LuPO4. Journal of Alloys and Compounds, 250,573.

Nipko, J. C., et. al. (1997). Lattice dynamics of xenotime: The phonon dispersion relations and density of states of LuPO4. Phys. Rev. B, 56,11584.

Rapaport, A., David, V., Bass, M., Deka, C., & Boatner, L. A. (1999, in press). Optical spectroscopy of erbium-doped lutetium orthophosphate. J. Lumin.

Rapaport, A., Moteau, O., Bass, M., Boatner, L. A., & Deka, C. (1999). Optical spectroscopy and lasing properties of neodymium-doped lutetium orthophosphate. Jornal of Optical Soc. Am. B, 16,911-916.

Publication Type: Paper

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1999, Apr. 25-28). Radiation effects in Lanthanide-bearing AB04 compounds proposed for nuclear waste disposal. Presentation at a special focused session on Lanthanide-Containing Materials and Applications at the American Ceramic Society 101st Annual Meeting. Indianapolis, IN.

Meldrum, A., Boatner, L. A., White, C. W., & Henderson, D. O. (1999). Radiation effects in nonmetals: Amorphization, phase decomposition, and nanoparticles. Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). Microstructural Processes in Irradiated Materials. Materials Research Symposium Proceedings, 540,135. Boston, MA.

Meldrum, A., et. al. (1999). Radiation effects in zircon, hafnon, and thorite: Implications for Pu disposal. Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). Microstructural Processes in Irradiated Materials. Materials Research Symposium Proceedings, 540,395. Boston, MA.

Meldrum, A., Zinkle, S. J., Boatner, L. A., & Ewing, R. C. (1999). Heavy-ion irradiation effects in the ABO4 orthosilicates: Decomposition, amorphization, and recrystallization. Physical Review B, 59,3981-3992.

Weber, W. J., et. al. (1999). The effect of temperature and damage energy on amorphization in zircon. Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). Microstructural Processes in Irradiated Materials. Materials Research Symposium Proceedings, 540,367. Boston, MA.

Publication Type: Presentation

Boatner, L. A. (1998, Mar. 5). Living in a materials world. Invited presentation for the induction seminar at the Academy of Sciences of Mexico. Mexico City, Mexico.

Boatner, L. A., Meldrum, A., Chakoumakos, B. C., & Mitchell, M. J. (1998, Sept. 11-12). The lanthanide orthophosphates: Chemically durable, radiation-resistant, high-temperature ceramics. Invited presentation at the Workshop on Advanced Materials for Extreme Environments: New Experimental Opportunities in Neutron Scattering. Argonne, IL.

Hanchar, J. M., Boatner, L. A., & Townsend, P. D. (1999, Apr. 25-28). Cathodoluminescence spectroscopy of the trivalent rare Earth elements in synthetic REEPO4, YPO4, and ScPO4. Presented at the American Ceramic Society 101st Annual Meeting. Indianapolis, IN.

Liu, G. K., et. al. (1997, Sep. 28 - Oct. 3). Self-radiation induced anisotropic structure damage in 244Cm-doped orthophosphate LuPO4. Presented at the 21st International Symposium on the Scientific Basis for Nuclear Waste Management, Davos Congress Center. Davos, Switzerland.

Loong, C. -K., Boatner, L. A., & Wang, J. Y. (1999, Jun. 20-23). Magnetic and thermodynamic properties of rare-Earth orthophosphates and pentaphosphates. Presentation at the 15th University Conference on Glass Science, University of Missouri. Rolla, MO.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1997, Dec. 1-5). Heavy-ion-irradiation of barium and strontium titanate: The effects of thermally-induced phase transitions and irradiation temperature. Presented at the Fall Meeting of the Materials Research Society, Symposium B: Phase Transformations and Systems Driven Far From Equilibrium. Boston, MA.

Meldrum, A., Boatner, L. A., Zinkle, S. J., & Ewing, R. C. (1999, Mar. 28 - Apr. 1). Ion irradiation effects in the zircon-structure orthosilicates. Presented at the 10th European Union of Geosciences. Strasbourg, France.

Meldrum, A., et. al. (1998, Nov. 30 - Dec. 4). Radiation effects in nonmetals: Amorphization, phase decomposition, and nanoparticles. Invited presentation at the 1998 Fall Materials Research Society Meeting. Boston, MA.

Meldrum, A., Ewing, R. C., & Boatner, L. A. (1997, Sep. 14-19). Effects of displacive and ionizing radiation on several perovskite-structure compounds. Presented at Radiation Effects in Insulators-9 (REI-9). Knoxville, TN.

Meldrum, A., Zinkle, S. J., Boatner, L. A., & Ewing, R. C. (1998, Aug. 31 - Sep. 4). Evidence for thermal spikes and cascade quenching in the zircon-structure orthosilicates. Presented at the Ion Beam Modification of Materials-98. Amsterdam, Netherlands.

Sales, B. C., Boatner, L. A., & Ramey, J. O. (1999, Jun. 20-23). Chromatographic studies of the structures of amorphous phosphates: A review. Presentation at the 15th University Conference on Glass Science, University of Missouri. Rolla, MO.

Trukhin, A. N. & Boatner, L. A. (1999, Aug. 16-20). Luminescence properties of ScPO4 single crystals. The 5th International Conference on Inorganic Scintillators and Their Applications, SCINT99, Moscow, Russia.

Weber, W. J., et. al. (1998, Nov. 30 - Dec. 4). The effect of temperature and recoil spectra on amorphization in zircon. Presented at the Fall Meeting of the Materials Research Society, Symposium N: Microstructural Processes in Irradiated Materials. Boston, MA.

Weber, W. J., et. al. (1999, Aug. 23-25). Ion-beam-induced defects and defect interactions in perovskite-structure titanates. Defects and Surface-Induced Effects in Advanced Perovskites. NATO Advanced Research Workshop. Jurmala, Latvia.

Publication Type: Theses/Dissertations

Meldrum, A. (1999). Radiation effects in the orthophosphates. PhD dissertation at the Department of Earth Sciences, University of New Mexico. Albuquerque, NM.

Project: 55100

Title: Human Genetic Marker for Resistance to Radiations and Chemicals
PI: Dr. Howard B. Lieberman *Institution:* Columbia University

Publication Type: Journal

Hang, H., Rauth, S. J., Hopkins, K. M., Davey, S. K., & Lieberman, H. B. (1998). Molecular cloning and tissue-specific expression of Mrad9, a murine orthologue of the Schizosaccharomyces pombe rad9+ checkpoing control gene. J. Cell Physiol., 177,232-240.

Project: 55103

Title: Utilization of Kinetic Isotope Effects for the Concentration of Tritium
PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Barton, J. W., Klasson, K. T., & Davison, B. H. (1997). Extended operation and control of biomass overgrowth in biofiliters designed for VOC removal. Proceedings of the 90th Annual Meeting & Exhibition of Air and Waste Management Association. Toronto, Ontario, Canada.

Huynh, M. H. V., et. al. (1999). Oxo-like reactivity of high oxidation state osmium hydrazido complexes. Journal of American Chemical Society, 121,1403-1404.

Huynh, M. H. V., White, P. S., & Meyer, T. J. (1999, in press). Proton-coupled electron transfer from nitrogen: A N-H/N-D Kinetic Isotope Effect of 41.4". Journal of American Chemical Society.

Lebeau, E. L. & Meyer, T.J. (1999). Oxidation of benzyl alcohol by a dioxo complex of Ru(VI). Inorganic Chemistry, 38,2174-2181.

Trammell, S. A., et. al. (1998). Mechanisms of surface electron transfer: Proton-coupled electron transfer. Journal of American Chemical Society, 120,13248-13249.

Project: 55108

Title: Monitoring Genetic & Metabolic Potential for In Situ Bioremediation: Mass Spectrometry

PI: Dr. Michelle V. Buchanan *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Costello, A. M. & Lidstrom, M. E. (1999, in press). Molecular characterization of functional and phylogenetic genes from natural populations of methanotrophs in lake sediments. Appl. Env. Microbiol.

Hurst, G. B., et. al. (1998). MALDI-TOF analysis of polymerase chain reaction products from methanotrophic bacteria. Analytical Chemistry, 70,2693-2698.

Publication Type: Poster

Hurst, G. B., et. al. (1998, Jan. 24-27). TOF-MS detection of PCR products. Poster presentation at the 10th Sanibel Conference on Mass Spectrometry, Sanibel Island, FL.

Hurst, G. B., Kim, Y., Weaver, K., & Buchanan, M. V. (1999, Jan. 12-16). PCR product size measurement using MALDI mass spectrometry. Poster presentation at the 7th DOE Human Genome Contractor-Grantee Workshop. Oakland, CA.

Publication Type: Presentation

Buchanan, M. V., et. al. (1998, Jul. 27-30). Monitoring genetic and metabolic potential for in situ bioremediation: Mass spectrometry. Presentation at the DOE Environmental Management Science Program Workshop, Chicago, IL.

Hurst, G. B. (1999, Nov. 5-6). Characterization of bacteria using mass spectrometric detection of polymerase chain reaction products. Presentation at the 7th Symposium on Laser Spectoscopy at the Korea Atomic Energy Research Institute.

Hurst, G. B., Weaver, K., & Buchanan, M. V. (1997, Nov. 9-13). Improved mass spectrometric resolution for PCR product size measurement. Presentation at the DOE Human Genome Program Contractor-Grantee Workshop VI, Santa Fe, NM. 39.

Kim, Y., Hurst, G. B., Doktycz, M. J., & Buchanan, M. V. (1999, Jun. 13-18). Improved spot homogeneity for DNA MALDI matrices. Presentation at the 47th ASMS Conference on Mass Spectrometry and Allied Topics. Dallas TX.

Publication Type: Proceeding

Hurst, G. B., et. al. (1998, May 31 - Jun. 4). Identification of methanotrophic bacteria using the polymerase chain reaction with MALDI-TOF detection. Proceedings of the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando FL. 1202.

Hurst, G. B., Weaver, K., Buchanan, M. V., & Doktycz, M. J. (1997, Jun. 1-5). Analysis of PCR products using delayed-extraction MALDI-TOF. Proceedings of the 45th ASMS Conference on Mass Spectrometry and Allied Topics. Palm Springs, CA. 843.

Weaver, K., Doktycz, M. J., Britt, P. F., Hurst, G. B., & Buchanan, M. V. (1998, May 31 - Jun. 4). 96-well microtiter-format purification of DNA for MALDI-TOF analysis. Proceedings of the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando FL. 1017.

Publication Type: Theses/Dissertations

Auman, A. (1999). Soluble methane monooxygenase-containing methanotrophs in lake Washington. Lidstrom, M. E. (Advisor). PhD dissertation at the Microbiology Department, University of Washington. Seattle, WA.

Costello, A. (1999, Apr.). Characterization of methanotrophic populations in lake Washington. Lidstrom, M. E. (Advisor). PhD dissertation at the California Institute of Technology, Environmental Engineering Science Department.

Project: 55110

Title: An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms

PI: Dr. Delbert E. Day *Institution:* University of Missouri-Rolla

Publication Type: Journal

Day, D. E. (1997). Structural features of iron-phosphate glasses. J. Non-Cryst. Solids, 222,144.

Day, D. E. (1997). Structural study of iron phosphate glasses. Phys. Chem. Glasses, 38,74.

Day, D. E. (1998). Chemically durable iron phophate glass wasteforms. J. Non-Cryst. Solids, 241,1.

Day, D. E. (1998). On the structure and radiation chemistry of iron phosphate glasses: New insights from electron spin resonance and evolved gas mass spectroscopy. Nucl. Inst. Meth. Phys. Res. B, 141,600.

Day, D. E. (1998). Redox characteristics and structural properties of iron phosphate glasses: A potential host matrix for vitrifying high level nuclear waste. Ceramic Transactions, 87,261.

Publication Type: Proceeding

Day, D. E. (1999). Effects of nuclear waste components on redox equilibria, structural features, and crystallization characteristics of iron phosphate glasses. Environment Issues and Waste Management Technologies IV: Ceramic Transactions, 93,195.

Day, D. E. (1999). Iron redox equilibria and crystallization of iron phosphate glasses. Environment Issues and Waste Management Technologies IV: Ceramic Transactions, 93,187.

Project: 55118

Title: Plant Rhizosphere Effects on Metal Mobilization and Transport
PI: Dr. Teresa W. M. Fan *Institution:* University of California at Davis

Publication Type: Journal

Fan, T. W. -M., Pedler, J., Lane, A. N., Crowley, D., & Higashi, R. M. (1997). Comprehensive analysis of organic ligands in whole root exudates using NMR and GC-MS. Analytical Biochemistry, 251,57-68.

Higashi, R. M., Fan, T. W. -M., & Lan, A. N. (1998). Association of desferrioxamine with humic substances and their interaction with cadmium(II) as studied by pyrolysis gas chromatography mass spectrometry and nuclear magnetic resonance spectroscopy. Analyst, 123(5),911-918.

Publication Type: Other

Fan, T. W. -M. & Lane, A. N. (1999, in press). NMR in the plant-soil environment. In Encyclopedia of NMR Spectroscopy, John Wiley and Sons, New York, NY.

Fan, T. W. -M. (1996). Recent advancement in profiling plant metabolites by multi-nuclear and multi-dimensional NMR. In Shachar-Hill, Y., & Pfeffer, P. E. (Eds.), Nuclear Magnetic Resonance in Plant Biology. American Society of Plant Physiologists. Rockville, MD. 181-254.

Publication Type: Presentation

Fan, T. W. -M., Higashi, R. M., & Crowley, D. E. (1998, Jul.). Plant rhizosphere effects on metal mobilization and transport. DOE EMSP Symposium, Chicago, IL.

Fan, T. W. -M., Shenker, M., Higashi, R. M., Crowley, D. E., & Lane, A. N. (1999, Mar.). Rhizosphere mobilization of heavy metals via plant root exudation. Semi-Annual Meeting of American Chemical Society, Anaheim, CA.

Fan, T. W. -M., Shenker, M., Lane, A. N., Crowley, D., & Higashi, R. M. (1998, Apr.). Comprehensive determination of root exudates under combined Fe deficiency/CD stress by NMR and GC-MS. Society of Environmental Toxicology and Chemistry-Europe. Bordeaux, France.

Higashi, R. M. & Fan, T. W. -M. (1998, May). Ternary interactions of Cd(II), ligands, and humic substances - implications for metal ion bioavailability. EPA, DOE, ONR, & NSF Joint Workshop.

Higashi, R., Fan, T., Baraud, F., & Lane, A. (1999, Mar.). Ternary interactions of biogenic ligands and Cd(II) with humic substances, with implications for metal ion bioavailability. Semi-annual meeting of the American Chemical Society, Anaheim, CA.

Project: 55119

Title: Phase Equilibria Modification by Electric Fields
PI: Dr. Costas Tsouris *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Blankenship, K. D., DePaoli, D. W., Hylton, J. O., & Tsouris, C. (1999). Effect of electrode configurations on phase equilibria with electric fields. Separation and Purification Technology, 15,283-294.

Blankenship, K. D., Shah, V. M., & Tsouris, C. (1999). Distillation under electric fields. Separation Science and Technology, 34,1393-1409.

Norato, M. A., Tsouris, C., & Tavlarides, L. L. (1998). Phase inversion studies in liquid-liquid dispersions. The Canadian Journal of Chemical Engineers, 76,486-494.

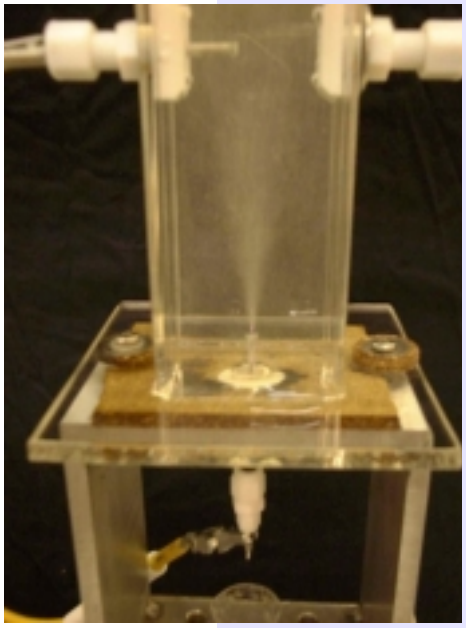
Shin, W-. T., Yiacoumi, S., & Tsouris, C. (1997). Experiments on electrostatic dispersion of air in water. Industrial and Engineering Chemistry Research, 36,3647-3655.

Tsouris, C. W., Shin, T., Yiacoumi, S., & DePaoli, D. W. (1999, in press) Effects of electric fields on bubble and particle velocities in water and alcohols. Journal of Colloid and Interface Science.

Tsouris, C., Borole, A. P., & Kaufman, E. N., DePaoli, D. W. (1999). An electrically driven gas-liquid-liquid contactor for bioreactor and other applications. Industrial and Engineering Chemistry Research, 38, 1877-1883.

Tsouris, C., DePaoli, D. W., & Yiacoumi, S., (1999, Jun. 1). Novel environmental technologies driven by electric and magnetic fields. Environmental Technologies and Opportunities Forum. Oak Ridge, TN.

Tsouris, C., Shin, W.- T. & Yiacoumi, S. (1998). Pumping, spraying, and mixing of fluids by electric fields. The Canadian Journal of Chemical Engineers, 76,589-599.



Simultaneous pumping, spraying, and mixing of a gas in an aqueous solution by means of an electric field can be used for the removal of contaminants from the solution. [see Project #55119]

Publication Type: Paper

Tsouris, C., & Dong, J. (1999, Jun. 13-16). Electric-effects on fluid interfaces. 73rd ACS Colloid and Surface Science Symposium, Massachusetts, Institute of Technology. Cambridge, MA.

Publication Type: Theses/Disseratations

Blankenship, K. D. (1999, Apr.). Distillation with applied electric fields. Master Thesis, Department of Chemical Engineering, University of Tennessee. Knoxville, TN.

Project: 55179

Title: Acoustic Probe for Solid-Gas-Liquid Suspensions
PI: Dr. Lawrence L. Tavlarides *Institution:* Syracuse University

Publication Type: Journal

Spelt, P. D. M., Norato, M. A., Sangani, A. S., & Tavlarides, L. L. (1999). Determination of particle size distributions from acoustic wave propagation measurements. Phys. Fluids, 11,1065-1080.

Project: 55188

Title: Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation
PI: Dr. David L. Griscom *Institution:* Naval Research Laboratory

Publication Type: Journal

Griscom, D. L., Merzbacher, C. I., Weeks, R. A., & Zuhr, R. A. (1999). Electron spin resonance studies of defect centers induced in a high-level nuclear waste glass simulant by gamma-irradiation and ion-implantion. J. Non-Cryst. Solids 258,34-47.

Project: 55196

Title: In Situ, Field Scale Evaluation of Surfactant Enhanced DNAPL Recovery Using a Single-Well, Push-Pull Test
PI: Dr. Jonathan D. Istok *Institution:* Oregon State University

Publication Type: Journal

Field, J. A., Istok, J. D., Schroth, M. H., Sawyer, T. E., & Humphrey, M. D. (1999, in press). Laboratory investigation of surfactant-enhanced TCE solubilization using single-well, 'push-pull' tests. Ground Water.

Field, J.A., & Istok, J. D. (1999). Comment on estimation of nonaqueous phase liquid-water interfacial areas in porous media following mobilization by chemical flooding. Environmental Science and Technology, 32(2),3836-3837.

Istok, J. D., Field, J. A., Schroth, M. H., Sawyer, T. E., & Humphrey, M. D. (1999). Laboratory and field investigation of surfactant sorption ssing single-well 'push-pull' tests. Ground Water.

Project: 55218

Title: Seismic Surface-Wave Tomography of Waste Sites
PI: Dr. Timothy L. Long *Institution:* Georgia Institute of Technology

Publication Type: Other

Long, L. T. (1999, Feb.). Seismic surface wave tomography at waste sites. Research Note in Fast Times, the EEGS Newsletter.

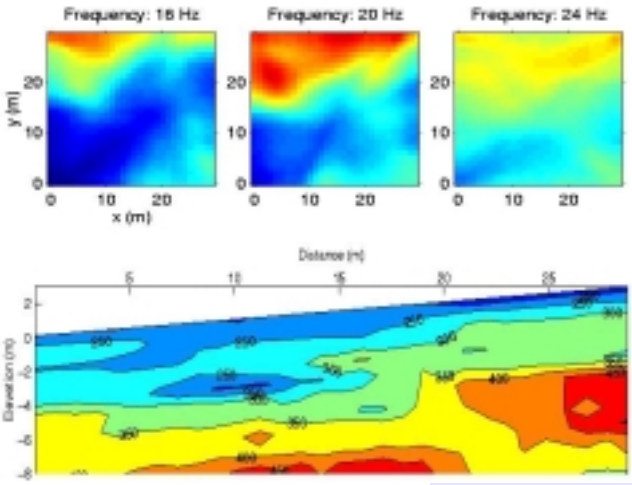
Publication Type: Paper

Long, L. T. & Kocaoglu, A. (1999, Oct. 16-20). A tomographic inversion method for near-surface structure. Eastern Section Seismological Society of America Annual Meeting. Memphis, TN.

Long, L. T., Kocaoglu, A., Doll, W. E., Chen, X. Q., & Martin, J. (1999, Oct.). Surface-wave group-velocity tomography for shallow structures at a waste site. SEG Expanded Abstract, Annual Meeting. Houston, TX.

Publication Type: Proceeding

Long, L. T., & Kocaoglu, A. (1999, Mar.). Surface-wave group-velocity tomography for shallow structures. Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems, Environmental and Engineering Geophysical Society (SAGEEP99).



Ever wonder what is under here? Generate a set of Group Velocity images (upper right), then invert the dispersion curves at each position to get an image of the shear-wave structure (lower right). The low velocity at 10m and 4m depth is a suspected burial trench, or the high uplifted under 25m could indicate a thrust fault. [see Project #55218]

Project: 55267

Title: Containment of Toxic Metals and Radionuclides in Porous and Fractured Meda: Optimizing Biogeochemical Reduction Versus Geochemical Oxidation

PI: Dr. Philip M. Jardine *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Barnett, M. O., Jardine, P. M., Brooks, S. C., & Selim, H. M. (1999, in press). Adsorption and transport of U(VI) in subsurface media. Soil Sci. Soc. Am. J.

Brooks, S. C., Carroll, S. L., & Jardine, P. M. (1999). Sustained bacterial reduction of Co(III)EDTA in the presence of competing geochemical oxidation during dynamic flow. Environ. Sci. Technol., 33,3002-3011.

Fendorf, S. E., Jardine, P. M., Patterson, R. R., Taylor, D. L., & Brooks, S. C. (1999, in press). Pyrolusite surface transformations measured in real-time during the reactive transport of Co(II)EDTA. Geochim. Cosmochim. Acta.

Jardine, P. M., et. al. (1999). Fate and transport of hexavalent chromium in undisturbed heterogeneous soil. Environ. Sci. Technol., 33,2939-2944.

Jardine, P. M., et. al. (1999). Quantifying diffusive mass transfer in fractured shale bedrock. Water Resour. Res., 35,2015-2030.

Publication Type: Other

Jardine, P. M., Brooks, S. C., Wilson, G. V., & Sanford, W. E. (1999, in press). Basic research strategies for resolving remediation needs in contaminated fractured subsurface media. In Faybishenko, B. (Ed.), Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. American Geophysical Union, Geophysical Monograph Series.

Jardine, P. M., O'Brien, R., Wilson, G. V., & Gwo, J. P. (1998). Experimental techniques for confirming and quantifying physical nonequilibrium processes in soils. In Selim, H. M. & Ma, L. (Eds.), Physical Nonequilibrium in Soils: Modeling and Application. Ann Arbor Press, Inc. Chelsea, MI. 243-271.

Publication Type: Presentation

Brooks, S. C. & Barnett, M. O. (1999, in press). Uranium sorption to bacterial cells as a related to metal reduction capabilities in the presence of porous media. Appl. and Eniron. Micro.

Brooks, S. C., & Jardine, P. M. (1997, Oct. 26-31). Bacterial reduction of toxic metals during dynamic flow. American Society of Agronomy. Anaheim, CA.

Guha, H., Saiers, J. E., Jardine, P. M., & Brooks, S. C. (1998, Dec. 6-10). Development and evaluation of a mathematical model for oxidation, sorption, and transport of Co(II)EDTA 2-. American Geophysical Union. San Francisco, CA.

Jardine, P. M. (1997, Apr. 13). Sorption induced inhibition of redox reaction involving manganese oxides. American Chemical Society. San Francisco, CA.

Jardine, P. M. (1997, Oct. 12). Geochemical processes governing the fate and transport of Cr(III) and Cr(VI) in soils. Soil Science Society of America. Anaheim, CA.

Jardine, P. M. (1997, Oct. 26). Bacterial reduction of toxic metals during dynamic flow. Science Society of America. Anaheim, CA.

Jardine, P. M., et. al. (1999, Feb. 6-10). Basic research strategies for resolving remediation needs in contaminated fractured subsurface media. Symposium on Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Lawrence Berkeley National Laboratory. Berkeley, CA.

Jardine, P. M., Wilson, G. V., Luxmoore, R. J., & Gwo, J. P. (1999, in press). Conceptual model of vadose-zone transport in fractured weathered shales. Hsieh, P. A. (Ed.), Conceptual Models of Flow and Transport in the Fractured Vadose Zone. National Research Council.

Jardine, P. M., Wilson, G. V., Sanford, W. E., & Luxmoore, R. J. (1998, May 14-16). Exploring subsurface transport mechanisms in fractured media at laboratory and field scales. Conference on “Mass transport in fractured aquifers and aquitards” Geological Institute, Unversity of Copenhagen, Denmark.

Mayes, M. A., Reedy, O. C., Larsen, I. L., Brooks, S. C., & Jardine, P. M. (1997,Oct. 26-31). Multispecies contaminant transport in undisturbed columns of weathered fractured shale. American Society of Agronomy. Anaheim, CA.

Mayes, M. A., Reedy, O. C., Larsen, I. L., Brooks, S. C., & Jardine, P. M. (1997, Oct.). Multispecies contaminant transport in undisturbed columns of weathered fractured shale. Geologic Society of America.

Mehlhorn, T. L., Jardine, P. M., Brooks, S. C., Fendorf, S. E., & Saiers, J. E. (1997, Oct. 26-31). Geochemical processes governing the fate and transport of Cr(III) and Cr(VI) in soils. American Society of Agronomy. Anaheim, CA.

Sanford, W. E., & Jardine, P. M. (1997, Oct. 26-31). Examining diffusion with multiple tracers to aid remediation of contaminated sites. American Society of Agronomy. Anaheim, CA.

Zhang, C., Brooks, S., Fendorf, S., & Jardine, P. (1998, Aug.). Microbial uranium reduction and biomineralization: Implication for immobilization of toxic metals and radionuclides. 17th Annual Meeting of the International Mineralogical Association. Toronto, Ontario, Canada.

Publication Type: Press release

Evans, R. & Hill, D. (1999). Press release initated by Department of Energy. One of 5 out of 200 EMSP projects to be featured in a press release package.

Norton, D. (1999, summer). Press release intiated by waste policy institute of Blacksburg, VA.

Publication Type: Proceeding

Fendorf, S. E., Jardine, P. M., Taylor, D. L., & Brooks, S.C. (1999). Auto-inhibition of oxide mineral oxidative capacity toward Co(II)EDTA: Time-resolved studies using XANES spectroscopy. In Sparks, D. L. & Grundel, T. (Eds.), Kinetics and mechanisms of sorption processes at the mineral-water interface. ACS Symposium Series 715,358-371.

Jardine, P. M. (1998, Aug. 24-28). Can basic research on contaminant transport be used to improve the design of remedial strategies? Proceedings of "School of Environmental Science and Technology". Buenos Aires, Argentina.

Jardine, P. M. (1998, Dec. 31). Auto-inhibition of oxide mineral oxidation capacity toward Co(II) EDTA: Time-resolved studies using XANES spectroscopy. In Sparks, D. L., & Grundel, T. (Eds.), Kinetics and mechanisms of sorption processes at the mineral-water interface. ACS Symposium Series.

Publication Type: Theses/Dissertations

Bostick, B. (1997). Pyrite chemistry in soils and waters: Reactivity toward radionuclides and heavy metals. Master's Thesis. Soil Science, University of Idaho. Moscow, ID.

Bostick, B. (Projected 2001). Sulfide and carbonate mineral adsorption processes of oxo-ions. Ph. D. candidate. Geological and Environmental Sciences, Stanford University. Palo Alto, CA.

Patterson, R. R. (1996). Iron sulfide reduction of chromate. Master's Thesis. Soil Science, University of Idaho. Moscow, ID.

Project: 55276

Title: Fundamental Chemistry and Thermodynamics of Hydrothermal Oxidation Processes

PI: Dr. John M. Simonson *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Blencoe, J. G., Anovitz, L. M., & Seitz, J. C. (1998, in press). A new method for modeling the thermodynamic mixing properties of high-temperature H2 O-CO2 fluids. Eos,79.

Blencoe, J. G., Seitz, J. C., & Anovitz, L. M., (1999, in press). The CO2 -H2 O System. II. Calculated Thermodynamic Mixing Properties for 400°C, 0-400 MPa. Geochim. Cosmochim. Acta, 63.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1998). Thermodynamics and kinetics of ion speciation in supercritical aqueous solutions: A molecular-based study. Fluid Phase Equilibria 150-151,107-115.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1999). Solvation in high-temperature electrolyte solutions. I. Hydration shell behavior from molecular simulation. J. Chem. Phys. 110,1064-1074.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1999). Solvation in high-temperature electrolyte solutions. II. Some formal results. J. Chem. Phys. 110,1075-1086.

Dai, S., Burleigh, M., Simonson, J. M., Mesmer, R. E., & Xue, Z. -L. (1998). Application of chemometric methods in UV-Vis absorption spectroscopic studies of uranyl ion dimerization reaction in aqueous solutions. Radiochimica Acta 81,195-199.

Moore, R. C., Mesmer, R. E., & Simonson, J. M. (1997). The solubility of potassium carbonate in water between 384 and 529 K measured using the synthetic method. J. Chem. Eng. Data 42,1078-1081.

Seitz, J. C. & Blencoe, J. G. (1999, in press). The CO2 -H2 O System. I. Experimental Determination of Volumetric Properties at 400°C, 10-100 MPa. Geochim. Cosmochim. Acta, 63.

Publication Type: Presentation

Blencoe, J. G., Anovitz, L. M. & Seitz, J. C. (1998). A Helmholz free energy model for supercritical H2 O-CO2 mixtures. Geol. Soc. Amer. Abs. with Prog., 30,A-319.

Blencoe, J. G., Anovitz, L. M., Seitz, J. C. (1997). Serious shortcomings of semi-empirical equations of state for high-temperature aqueous C-O-H-N fluids. Geol. Soc. Amer. Abs. with Prog. 29,A-210.

Seitz, J. C. & Blencoe, J. G. (1997). Experimentally determined volumetric properties and solvus relations for H2 O-CO2 -N2 mixtures at 300°C and pressures < 1000 bars. Geol. Soc. Amer. Abs. with Prog. 29,A-209.

Singh, J., Blencoe, J. G., & Seitz, J. C., (1998). Experimentally determined excess molar volumes for H2 O-N2 fluids at 300°C, 75-1000 bars. Geol. Soc. Amer. Abs. with Prog., 30,A-319.

Project: 55278

Title: Molecular Genetics of Metal Detoxification: Prospects for Phytoremediation
PI: Dr. David W. Ow *Institution:* U.S. Dept. of Agriculture

Picture 1 - shows a set of plants grown in high zinc concentration. Control plant (C) produces low biomass and suffers severe stress, as indicated by early flowering. In contrast, plants transgenic for genes Bj4 and Bj6 show healthy growth. [see Project #55278]

Publication Type: Journal

Ow, D. W. (1996). Heavy metal tolerance genes: Prospective tools for bioremediation. Resources, Conservation, and Recycle 18,135-149.

Perego, P., VandeWeghe, J., Ow, D. W., & Howell, S. B. (1997). The role of determinants of cadmium sensitivity in the tolerance of Schizosaccharomyces pombe to cisplatin. Molecular Pharmacology 51,12-18.

VandeWeghe, J. & Ow, D. W. (1999). A fission yeast gene for mitochondrial sulfide oxidation. Journal of Biological Chemistry, 274,13250-13257.

Publication Type: Other

Ow, D. W. (1998). Prospects of engineering heavy metal detoxification genes in plants. In Shewry, P. (Ed.), Engineering Crops for Industrial Uses. Portland Press. 111-124.

Publication Type: Presentation

Ow, D. W. (1996, Sept. 16-18). Prospects of engineering heavy metal detoxification genes in plants. Abstracts of the Symposium on Engineering Crops for Industrial End Uses. Bristol, England.

Ow, D. W. (1997, Sept. 29 - Oct. 1). Heavy metal tolerance genes as tools for phytoremediation. Abstracts of the International Symposium on Environmental Engineering. Kyongju, Korea.

Ow, D. W., Clark, S., Henstrand, J., & Kim, J. (1998, Jun. 19-20). Molecular genetics of heavy metal tolerance. Abstracts of the University of Connecticut Agricultural Biotechnology Symposium, Storrs, CN.

Ow, D. W., et. al. (1997, Sept. 21-27). Heavy metal tolerance genes for phytoremediation. Abtracts of the 5th International Congress of Plant Molecular Biology, Singapore.

Ow, D. W., et. al. (1998, Jul. 27-30). Heavy metal tolerance genes. Abstracts of the DOE Environmental Remediation Meeting. Chicago, IL.

VandeWeghe, J. & Ow, D. W. (1996, Aug. 6-11). An oxidoreductase-like gene required for cadmium tolerance in Schizosaccharomyces pombe. Abstracts of the 1996 Yeast Genetics & Molecular Biology Meeting. Univ. of Wisconsin. Madison, WI. 309.

VandeWeghe, J., Ow, D. W. (1997, Apr. 7-8). A novel mitochrondrial oxidoreductase required for phytochelatin accumulation and cadmium tolerance in fission yeast. Abstracts of the Society for Experimental Biology Annual Meeting, Session on Metals and Genes. Canterbury, England. 80.

Zankel, T. C. & Ow, D. (1996, Mar. 17-23). Homologs of the human BTF3 and Wiskott-Aldrich syndrome proteins are involved in the metal stress response of S. pombe. Abstracts of the 1996 Keystone Symposium on Transcriptional Mechanisms. Taos, NM. 67.

Zankel, T. C., Ow, D. W. (1997, Mar. 31 - Apr. 6). A Schizosaccharomyces pombe homolog of the Wiskott-Aldrich syndrome protein is involved in stress adaptation and mating. Abstracts of the 1997 Keystone Symposium on Temporal and Spatial Determinants of Specificity in Signal Transduction, Keystone, CO.

Publication Type: Proceeding

Perego, P, Vandeweghe, J, Ow, D, & Howell, S B. (1997). Role of determinants of cadmium sensitivity in the sensitivity of Schizosaccharomyces pombe to cisplatin. Eighty-eighth Annual Meeting of the American Association for Cancer Research, San Diego, CA. Also in the proceedings of the American Association for Cancer Research Annual Meeting, 38,393.

Perego, P., VandeWeghe, J., Ow, D., & Howell, S. B. (1996, Apr. 20-24). Mechanisms of resistance to cisplatin (DDP) in Schizosaccharomyces pombe. 87th Annual Meeting of the American Association for Cancer Research. Washington, D. C. Proceedings of the American Association for Cancer Research Annual Meeting, 37,336.

Project: 55294

Title: Superconducting Open-Gradient Magnetic Separation for the Pretreatment of Radioactive or Mixed Waste Vitrification Feeds

PI: Richard D. Doctor *Institution:* Argonne National Laboratory

Publication Type: Paper

Doctor, R. D. (1997, Oct. 24). Superconducting open-gradient magnetic separation for the pre-treatment of radioactive or mixed-waste vitrification feeds. Tenth Symposium on Separation Science and Technology for Energy Applications.

Project: 55318

Title: Improved Analytical Characterization of Solid Waste Forms by Fundamental Development of Laser Ablation Technology

PI: Dr. Richard E. Russo *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Journal

Borisov, O. V., Mao, X. L., & Russo, R. E. (1999, in press). Laser ablation ICP/MS calibration based on binary Cu/Zn alloy standards. Spectrochimica Acta B.

Borisov, O. V., Mao, X. L., Ciocan, A. C., & Russo, R. E. (1998). Time resolved parametric studies of laser ablation using ICP-AES. Applied Surface Science 129,315.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1998). Effects of gas environment on pico-second laser ablation. Applied Surface Science 129,269.

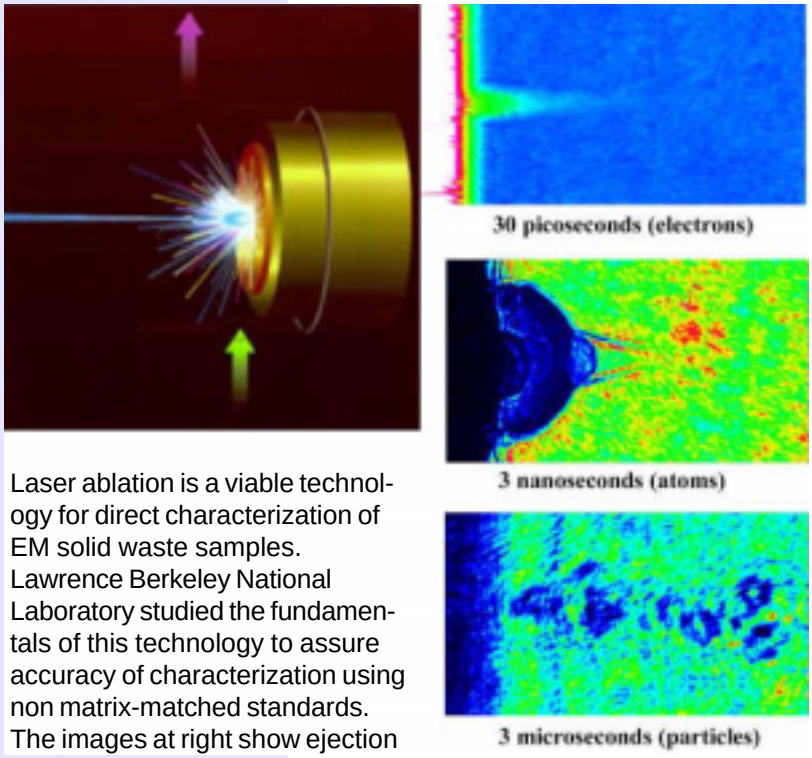
Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1998). Optical emission spectroscopy of the influence of laser ablated mass on dry inductively coupled plasma conditions. Spectrochimica Acta, 53B,463.

Leung, A. P. K., Chan, W. T., Mao, X. L., & Russo, R. E. (1998). Influence of gas atmosphere on picosecond laser ablation sampling efficiency and ICP-AES. Analytical Chemistry, 70(N22),4709.

Russo, R. E. (1998). Laser ablation sampling. Trends in Analytical Chemistry (Personal Edition), 17(8-9).

Russo, R. E. (1998, Jul. 1). Transient isotachophoretic - electrophoretic separations of lanthanides with indirect laser-induced fluorescence detection. Analytical Chemistry, 70(13).

Russo, R. E. (1998, Jul. 18). Preferential vaporization during laser ablation inductively coupled plasma atomic emission spectroscopy. Applied Spectroscopy, 52(7).



Laser ablation is a viable technology for direct characterization of EM solid waste samples. Lawrence Berkeley National Laboratory studied the fundamentals of this technology to assure accuracy of characterization using non matrix-matched standards. The images at right show ejection of electrons, atoms, and particles at different times during an ablation event. Understanding the contribution of each mass form to the chemical analysis is one of the goals of this research. [see Project #55318]

Russo, R. E. (1998, Mar. 30). Optical emission spectroscopy studies of the influence of laser ablated mass on dry inductively coupled plasma conditions. Spectrochimica Acta, Part B: Atomic Spectroscopy, 53(3).

Russo, R. E. (1998, May 29). Enhancements in laser ablation inductively coupled plasma-atomic emission spectrometry based on laser properties and ambient environment. Spectrochimica Acta, Part B: Atomic Spectroscopy, 53(5).

Russo, R. E. (1998, Nov. 15). Influence of gas environment on picosecond laser ablation sampling efficiency and ICP conditions. Analytical Chemistry, 70(22), Washington, D. C., 4709-4716.

Publication Type: Presentation

Borisov, O. V., Mao, X. L., & Russo, R. E. (1998, Oct.). Optimization of ICPMS for laser ablation sampling. 25th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Austin, TX.

Chan, W. -T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997, Oct.). Effect of gas medium on laser ablation sampling for ICP-AES. Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies. (FACSS). Providence, RI.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997, Jul.). Effects of gas atmosphere on pico-second laser ablation sampling for ICP-AES. Fourth International Conference on Laser Ablation (COLA 97). Asilomar, CA.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1997, Jul.). Optical emission spectroscopy of the influence of ablated material on dry inductively coupled plasma conditions. COLA 97. Asilomar, CA.

Russo, R. E. (1998, Sept.). Laser-ablation sampling with ICP/AES and ICP/MS: Fundamental issues to improve analytical applications. Invited presentation at the Society of Applied Spectroscopy California Section Meeting. Fremont, CA.

Russo, R. E. (1999, Apr.). Fundamental and applied aspects of laser ablation for chemical analysis. Frontiers in Chemistry Lecture Series. Wayne State University. Detroit, MI.

Russo, R. E., Jeong, S. H., Mao, X. L., Borisov, O. V., & Yoo, J. (1998, Oct.). Particle generation and transport during laser ablation sampling for chemical analysis. 25th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Austin, TX.

Russo, R. E., Mao, X. L., Ciocan, A. C., & Borisov, B. V. (1997, Oct.). Laser ablated mass influence on the properties of the ICP. Invited presentation at the Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies. (FACSS). Providence, RI.

Russo, R. E., Mao, X. L., Ciocan, A. C., & Borisov, B. V. (1997, Oct.). Laser ablation solid sample chemical analysis: Dream or reality. Invited presentation at the Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Providence, RI.

Publication Type: Proceeding

Borisov, O. V., Mao, X. L. & Russo, R. E. (1999, Apr.). Direct characterization of solid waste forms using laser ablation ICPMS. Waste Management Science and Technology in the Ceramic and Nuclear Industries. American Ceramic Society.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997). Effects of gas atmosphere on pico-second laser ablation sampling for ICP-AES. Fourth International Conference on Laser Ablation (COLA 97). Asilomar, CA.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1997, Jul.). Optical emission spectroscopy studies of ablated material on dry inductively coupled plasma conditions. COLA. Asilomar, CA.

Mao, X. L., Ciocan, A. C., Borisov, O. V., & Russo, R. E. (1997, Jul.). Time resolved parametric studies of laser ablation of brass using ICP-AES. COLA 97. Asilomar, CA.

Russo, R. E. (1997, Jul. 21-25). Effects of gas environment on picosecond laser ablation. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation, 127-129.

Russo, R. E. (1997, Jul. 21-25). Propagation of the shock wave generated from excimer laser heating of aluminum targets in comparison with ideal blast wave theory. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation.

Russo, R. E. (1997, Jul. 21-25). Time-resolved parametric studies of laser ablation using inductively coupled plasma atomic emission sectroscopy. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation.

Russo, R. E., Mao, X. L., & Borisov, O. V. (1998). Laser Ablation Sampling. Trends in Analytical Chemistry,17,461.

Project: 55328

Title: Novel Analytical Techniques Based on an Enhanced Electron Attachment Process

PI: Dr. Lal A. Pinnaduwage *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998). Enhanced negative ion formation by electron attachment to highly-excited molecules in a flowing plasma. J. Appl. Phys. 84,3051.

Ding, W., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999, in press). The role of high Rydberg states in enhanced O-formation in a pulsed O2 discharge. Plasma Sources Sci. Technol., 8,384.

Mabel, A. M., Lin, S. H., & Pinnaduwage, L. A. (1998). Potential energy surfaces of H2. Chem. Phys. Lett. 285,114.

Nagesha, K. & Pinnaduwage, L. A. (1998). O-formation from O2 via Rydberg-Rydberg electron transfer. J. Chem. Phys. 109,7124.

Nagesha, K. & Pinnaduwage, L. A. (1999, in press). Magnetic and electric field induced enhancements in laser induced anion formation. Chemical Physics Letters.

Pinnaduwage, L. A. & Zhu, Y. (1997). Long-time stability of superexcited high-Rydberg molecular states. Chem. Phys. Lett., 277,147.

Pinnaduwage, L. A. & Zhu, Y. (1998). High-Rydberg fragment formation via core dissociation of superexcited Rydberg molecules. J. Chem. Phys. 108, 6633.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999, in press). Enhanced electron attachment to highly-excited molecules and its applications in pulsed plasmas. Digest of Technical Papers of the 12th IEEE Pulsed Power Conference, IEEE Publishing Services, New York, NY.

Pinnaduwage, L. A., et. al. (1999). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. J. Appl. Phys., 85,7064.

Pinnaduwage, L. A., McCorkle, D. L., & Ding, W. (1997). Enhanced electron attachment to highly excited molecules using a plasma mixing scheme. Appl. Phys. Lett. 71,3634.

Pinnaduwage, L. A., Nagesha, K., Zhu, Y., Buchanan, M. V., & Hurst, G. B. (1999, in press). Laser-enhanced negative ion mass spectroscopy for weakly-electron-ataching species. Int. J. Mass Spectrom, Ion Processes.

Publication Type: Presentation

Ding, W. X., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999, Mar. 20-26). O formation by electron attachment to high Rydberg states. Presentation at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Nagesha, K. & Pinnaduwage, L. A. (1999, Oct. 5-8). Magnetic and electric field induced enhancements in laser induced anion formation. 52nd Annual Gaseous Electronics Conference. Norfolk, Virginia.

Pinnaduwage, L. A., Buchanan, M. V., & Hurst, G. B. (1998, Jul. 27-30). Novel analytical techniques based on an enhanced electron atachment process. Presented at the Environmental Management Science Program Workshop, Chicago, IL.

Pinnaduwage, L. A., Ding, W. & McCorkle, D. L. (1999, Oct. 5-8). Negative ion formation in pulsed plasmas. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Presentation at the 1998 International Congress on Plasma Physics. Prague, Czech Republic.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999, Mar. 20-26). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. Presentation at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999, Jun. 27-30). Implications of electron attachment to highly-excited states of molecules and its applications in pulsed plasmas. 12th IEEE Pulsed Power Conference. Monterey, CA.

Tav, C. & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociative electron attachment to laser-excited benzene. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Zhu, Y. & Pinnaduwage, L. A. (1997, Oct. 6-9). Long-time stability of superexcited high Rydberg molecular states. 50th Annual Gaseous Electronics Conference. Madison, WI.

Publication Type: Proceeding

Pinnaduwage, L. A, Ding, W. X., & McCorkle, D. L. (1999). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Pavlo, P. (Ed). Proceedings of the 1998 International Congress on Plasma Physics. Prague, Czech Republic. 129-132.

Pinnaduwage, L. A. (1997, Jun. 29 - Jul. 2). Implications of electron attachment to highly-excited states in pulsed power discharges. Cooperstein, G. & Vitkovitsky, I. (Eds.). Digest of Technical Papers of the 11th IEEE Pulsed Power Conference held in Baltimore, MD. IEEE Publishing Services, New York, NY. 1048-1053.

Publication Type: Theses/Dissertations

Tav, C. (projected summer 2000). Enhanced electron attachment to vibrationally and electronically excited molecules. PhD dissertation.

Project: 55332

Title: A Hybrid Hydrologic-Geophysical Inverse Technique for the Assessment and Monitoring of Leachates in the Vadose Zone
PI: James R. Brainard *Institution:* Sandia National Laboratories

Publication Type: Theses/Dissertations

Paprocki, L. T. (2000). Characterization of vadose zone in-situ moisture content and an advancing wetting front using cross-borehole ground penetrating radar. Master's Thesis. Department of Hydrology, New Mexico Institute of Mining and Technology. Socorro, New Mexico.

Yang, X. (1999). Stochastic inversion of 3-D ERT data. Ph. D. dissertation. Department of Mining and Geological Engineering, University of Arizona. Tucson, AZ.

Project: 55359

Title: Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone
PI: Dr. Boris Faybishenko
Institution: Lawrence Berkeley National Laboratory

Publication Type: Journal

Finsterle, S. & Faybishenko, B. (1999). Design and analysis of an experiment to determine hydraulic parameters of variably saturated porous media. Advances in Water Resources, 22(1),431-444.

Publication Type: Presentation

Carrigan, C. R, et. al. (1999). Lessons on transport and monitoring from the LLNL Vadose Zone Observatory. Proceedings of the 1999 Spring AGU Meeting. Boston, MA.

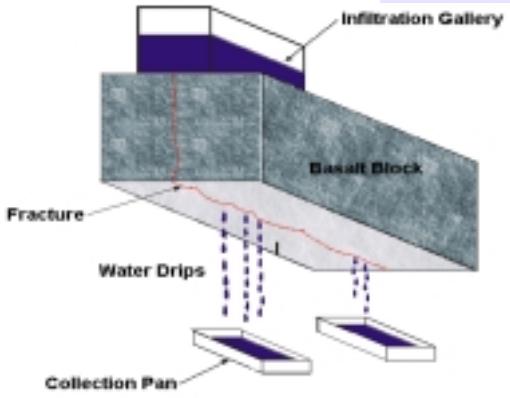


Illustration of the infiltration test design at the Hell's Half Acre site, Idaho, to investigate a key problem of infiltration in fractured rocks - water dripping through fractures. [see Project #55359]

Faybishenko, B. & Finsterle, S. (1999). On the physics of tensiometry in heterogeneous soils and rocks. Proceedings of the 1999 Spring AGU Meeting. Boston, MA.

Faybishenko, B. (1998, May). Theory and numerical evaluation of the parameters of the chaotic behavior of flow in unsaturated soils and rocks. Chapman Conference on Fractal Scaling, Non-Linear Dynamics, and Chaos in Hydrologic Systems. Clemson University. Clemson, SC.

Faybishenko, B. (1998, Oct.). A fuzzy-chaotic analysis of water flow and chemical transport in unsaturated-saturated soils. 16th World Congress of Soil Science. Montpellier, France.

Faybishenko, B. (Ed.) (1999, Feb. 10-12), Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA.

Faybishenko, B., et. al. (1997). Conceptual model of geometry and physics of liquid flow in unsaturated fractured basalt at Box Canyon Site. Proceedings of the 1997 Fall Meeting of AGU. San Francisco, CA.

Faybishenko, B., et. al. (1998). Multi-scale investigations of flow in fractured rocks. Proceedings of the 1998 Fall Meeting of AGU. San Francisco, CA. F377-378.

Faybishenko, B., Wood, T. R., Stoops, T. M., Doughty, C., & Jacobsen, J. (1997). A conceptual model of tracer transport in fractured basalt: Large Scale Infiltration Test revisited. Proceedings of 1997 GSA Annual Conference. Salt Lake City, UT.

Geller, J. T., Borglin, S. E., & Faybishenko, B. (1998). Experimental study and evaluation of dripping water in fracture models. Proceedings of the 1998 Fall Meeting of AGU. San Francisco, CA. F383.

Geller, J. T., Borglin, S. E., & Faybishenko, B. (1998, May). Experimental study and evaluation of dripping water in fracture models. Chapman Conference on Fractal Scaling, Non-Linear Dynamics, and Chaos in Hydrologic Systems. Clemson University. Clemson, SC.

Publication Type: Press release

Faybishenko, B. (1999, Dec. 17). Water travels chaotically through the ground. A Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone (see Web site: http: // www.eurekalert.org/releases/ineel-wtcttg.html).

Publication Type: Proceeding

Faybishenko, B. (1999). Comparison of laboratory and field methods for determination of unsaturated hydraulic conductivity of soils. LBNL Report-42022. Proceedings of the International Conference - Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media.

Faybishenko, B. (1999). Evidence of chaotic behavior in flow through fractured rocks, and how we might use chaos theory in fractured rock hydrogeology. In Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA. 207-212.

Finsterle, S. & Faybishenko, B. (1998). What does a tensiometer measure in fractured rocks? LBNL Report-41454. Proceedings of the International Conference - Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media.

Nikravesh, M., Cox, L., Faybishenko, B., & Aminzadeh, F. (1999, Mar.). Characterization of contaminated sites using sparse well data. SPE Paper 49330.

Podgorney, R. K. & Wood, T. R. (1999). Observations of water movement in variably saturated fractured basalt and its possible implications on predictive modeling. In Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA. 300-304.

Publication Type: Report

Babchin, A. J., Faybishenko, B., Sivashinsky, G. I., Frenkel, A., & Halpern, D. (1999). A model of chaotic time evolution of a slow liquid film on an inclined plane: One-dimensional solution. LBNL Report 42884.

Benito, P., Cook, P., Faybishenko, B., Freifeld, B., & Doughty, C. (1999). Box canyon air-connectivity study. Preliminary Data Analysis, LBNL Report 42359.

Faybishenko, B., et al. (1997). A chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone. In Environmental Management Science Program Awards Fiscal Year 1997 Annual Report Progress. Lawrence Berkeley National Laboratory Report, LBNL-41192.

Faybishenko, B., et. al. (1997). A chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone. 1997 Annual Report. Report No. LBNL-41223.

Podgorney, R. K., Wood, T. R., & Stoops, T. M. (1998). Basalt outcrop infiltration tests to evaluate chaotic behavior of unsaturated flow in fractured rock. INEEL Data Summary Report 1997 Field Season.

Podgorney, R. K., Wood, T. R., & Stoops, T. M. (1999). Basalt outcrop infiltration tests to evaluate chaotic behavior of unsaturated flow in fractured rock. INEEL Data Summary Report 1998 Field Season.

Project: 55367

Title: Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques

PI: Dr. Guokui Liu *Institution:* Argonne National Laboratory

Publication Type: Journal

Liu, G. K., Li, S. T., Beitz, J. V., & Abraham, M. M. (1998). J. Alloys & Compounds, 271/273,872.

Publication Type: Proceeding

G. K. Liu, et. al. (1998). Scientific basis for nuclear waste management XXI. MRS Sym. Pro. V506, 921.

Project: 55380

Title: In-Situ Spectro-Electrochemical Studies of Radionuclide Contaminated Surface Films on Metals and the Mechanism of their Formation and Dissolution

PI: Dr. Carlos A. Melendres *Institution:* Argonne National Laboratory

Publication Type: Paper

Carlos, A. (1999, Apr. 5). X-ray absorption spectroscopy studies of electrochemically deposited thin oxide films. Materials Research Society Spring Meeting.

Melendres, C. A. (1999, May 3). X-ray absorption spectroscopy studies of the structure of electrodeposited metal oxide films and some applications. 193rd Meeting of the Electrochemical Society.

Project: 55388

Title: Stable Isotopic Investigations of In Situ Bioremediation of Chlorinated Organic Solvents

PI: Dr. Neil C. Sturchio *Institution:* Argonne National Laboratory

Publication Type: Journal

Heraty, L. J., Fuller, M. E., Huang, L., Abrajano, T., & Sturchio, N. C. (1999, in press). Carbon and chlorine isotopic fractionation during microbial degradation of dichloromethane. Organic Geochemistry.

Holt, B. D., Sturchio, N. C., Abrajano, T. A., & Heraty, L. J. (1997). Conversion of chlorinated organic compounds to carbon dioxide and methyl chloride for isotopic analysis of carbon and chlorine. Analytical Chemistry 69,2727-2733.

Huang, L., Sturchio, N. C., Abrajano, T., Heraty, L. J., & Holt, B. D. (1999, in press). Comparison of C and Cl isotope fractionation of chlorinated aliphatic hydrocarbons during evaporation and biodegradation. Organic Geochemistry.

Sturchio, N. C., et. al. (1998). Stable chlorine isotope investigation of natural attenuation of trichloroethene in an aerobic aquifer. Environmental Science and Technology 32,3037-3042.

Publication Type: Patent

Holt, B. D. & Sturchio, N. C. Method for isotopic analysis of chlorinated organic compounds. US5942439.

Project: 55395

Title: Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities

PI: Dr. Stephen H. Conrad *Institution:* Sandia National Laboratories

Publication Type: Report

Borchers, B., Conrad, S. H., Webb, E. K., Glass Jr., R. J., Cox, R. (1997). A simulation and decision analysis approach to locating DNAPL in subsurface sediments. Sandia Report SAND97-2261.

Project: 55411

Title: Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring

PI: Dr. Patricia A. Berge *Institution:* Lawrence Livermore National Laboratory

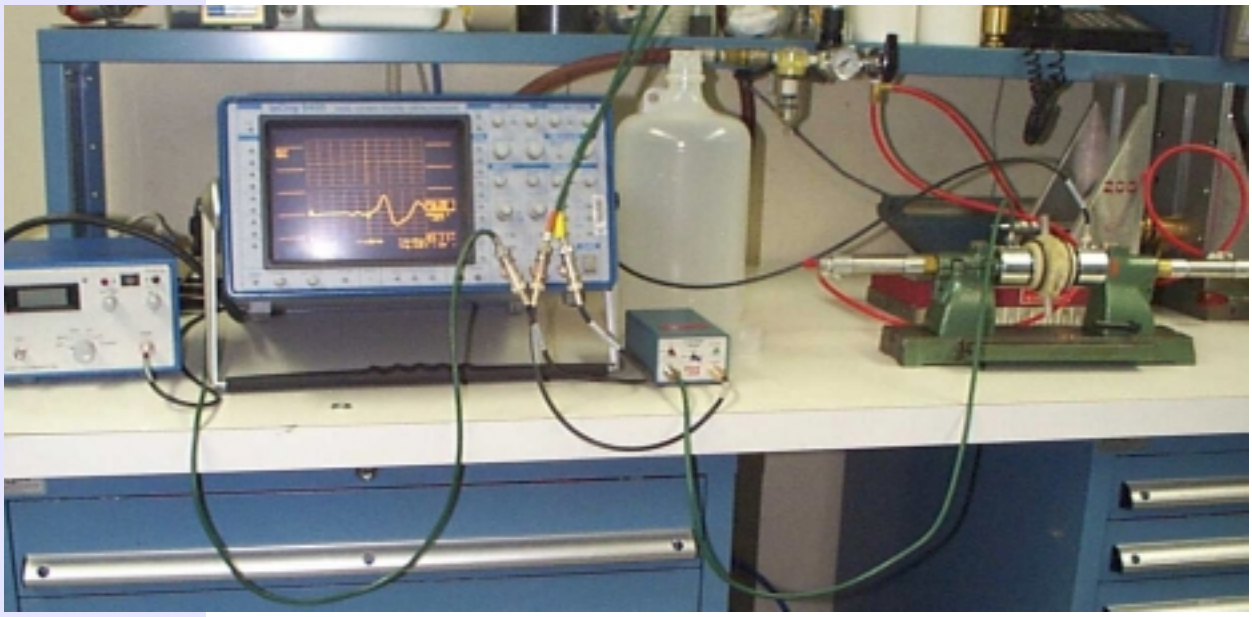
Publication Type: Journal

Berryman, J. G. & Pride, S. R. (1998). Volume averaging, effective stress rules, and inversion for microstructural response of multicomponent porous media. LLNL report UCRL-JC-127248, Int. J. Sol. Struct., 35,4811-4843.

Pride, S. R. & Berryman, J. G. (1998). Connecting theory to experiment in poroelasticity. J. Mech. Phys. Sol., 46,719-747.

Publication Type: Paper

Berryman, J. G. & Berge, P. A. (1999, Mar. 24-27). Mixture theory for predicting geomechanical coefficients of heterogeneous reservoirs. Fifth Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX. 110.



Photograph of experimental apparatus for measuring ultrasonic compressional and shear wave velocities in soils at low pressures. The oscilloscope screen displays an amplified signal from the pulse generator at the far left. This signal travelled through the soil sample in the sample holder assembly to the right. [see Project #55411]

Publication Type: Patent

Berryman, J.G. (1999). Robust discrimination of porosity and fluid saturation using seismic velocity analysis. DOE Patent Docket No. S-92015, LLNL Patent disclosure IL-10437.

Bonner, B. P., Boro, C., & Hart, D. J. (1999, Apr.). Anti-waveguide for ultrasonic testing of granular media under elevated stress. LLNL Patent disclosure.

Publication Type: Proceeding

Berge, P. A., Bonner, B. P., Aracne-Ruddle, C., Trombino, C., & Berryman, J. G. (1999). Compressional and shear wave velocities of soils at low pressures— Theoretical estimates, and comparison of laboratory and field data. LLNL report UCRL-JC-133211 Abs, Proceedings of the Seismological Society of America (SSA) 94th Annual Meeting, Seismological Research Letters, 70,226.

Bonner, B. P., et. al. (1999, Mar. 14-18). Ultrasonic characterization of synthetic soils for application to near surface geophysics. In Powers, M. H., Cramer, L., & Bell, R. S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 455-463.

Publication Type: Report

Aracne-Ruddle, C., Wildenschild, D., Bonner, B., & Berge, P. (1998). Direct observation of morphology of sand-clay mixtures with implications for mechanical properties in sediments. LLNL report UCRL-JC-131702 Abs, Eos, Transactions of the American Geophysical Union, 79, Fall Meeting Supplement, F820.

Aracne-Ruddle, C., Wildenschild, D., Bonner, B., & Berge, P. (1998, Oct. 15-16). Direct observation of fluid-clay interactions with implications for mechanical and electrical properties. LLNL report UCRL-JC-131116 Abs. Presentation at the LLNL Women's Technical and Professional Symposium. San Ramon, CA.

Berge, P. A. & Berryman, J. G. (1999, Mar. 24-27). Developing rock physics algorithms for velocity-porosity relations with environmental geophysics applications. LLNL report UCRL-JC-132054 Abs, Fifth Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX. 108.

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1999, Mar. 14-18). Comparing geophysical measurements to theoretical estimates for soil mixtures at low pressures. LLNL report UCRL-JC-132893. In Powers, M. H., Cramer, L., & Bell, R. S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP), Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 465-472.

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1998, Oct. 15-16). Preliminary results from an environmental geophysics Project: for improving geophysical imaging of fluid distribution in the shallow subsurface. LLNL report UCRL-JC-131209 Abs. Presentation at the LLNL Women's Technical and Professional Symposium. San Ramon, CA.

Berge, P. A., Berryman, J. G., Roberts, J. J., & Wildenschild, D. (1997). Joint inversion of geophysical data for site characterization and restoration monitoring. In Carrigan, C. R. & Jackson, K. J. (Eds.), Environmental Management Science Program: Fiscal Year 1997 Progress Report, Lawrence Livermore National Laboratory (LLNL) report UCRL-ID-129562, LLNL, Livermore, CA.

Berge, P. A., Berryman, J. G., Roberts, J. J., & Wildenschild, D. (1998, Jul. 27-30). Joint inversion of geophysical data for site characterization and restoration monitoring. EMSP Project: summary/progress report for FY98 for EMSP Project: 55411. LLNL report UCRL-JC-128343, presented at the DOE Environmental Management Science Workshop, Chicago, IL.

Berryman, J., Dvorkin, J., Le Ravalec, M., & Nur, A. (1997). Effective moduli of particulates with elastic cement. LLNL report UCRL-JC-128340.

Bonner, B. P., Hart, D. J., Berge, P. A., & Aracne, C. M. (1997). Influence of chemistry on physical properties: Ultrasonic velocities in mixtures of sand and swelling clay. LLNL report UCRL-JC-128306abs, Eos, Transactions of the American Geophysical Union, 78, Fall Meeting Supplement, F679.

Rowe, C. D. (1997, summer). Joint inversion of geophysical data for site characterization and restoration monitoring. In Williams, B. (Ed.), The Associated Western Universities Summer Participant Program at the Lawrence Livermore National Laboratory, Summer 1997: LLNL report UCRL-ID-128721-97, LLNL. Livermore, CA. 75-78.

Trombino, C. N. (1998). Elastic properties of sand-peat moss mixtures from ultrasonic measurements. LLNL report UCRL-JC-131770. LLNL, Livermore, CA.

Understanding the chemical and microbial conditions in the subsurface helps identify potential treatment solutions. [see Project #55416]

Wildenschild, D., Roberts, J. J. & Carlberg, E. D. (1998). Transport and microstructural properties of sand-clay mixtures. LLNL report UCRL-JC-131703 Abs, Eos, Transactions of the American Geophysical Union, 79, Fall Meeting Supplement, F820.

Wildenschild, D., Roberts, J. J., & Carlberg, E. (1999, Mar. 14-18). Influence of microstructural properties on geophysical measurements in sand-clay mixtures. LLNL report UCRL-JC-131557. In Powers, M. H., Cramer, L., & Bell, R.S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 445-454.

Project: 55416

Title: Control of Biologically Active Degradation Zones by Vertical Heterogeneity: Applications in Fractured Media

PI: Dr. Frederick S. Colwell

Institution: Idaho National Engineering and Environmental Laboratory

Publication Type: Poster

Colwell, F. S. (1999, Jan. 15). Control of biologically active degradation zones by vertical heterogeneity: Applications in fractured media. NABIR Investigator's Workshop.

During a tour of the INEEL Research Center labs, INEEL scientist Rick Colwell explained to DOE Deputy Secretary T.J. Glautheir, DOE-Idaho Manager Bev Cook, Merna Hurd, senior adviser for Glautheir, and Linda McCoy, DOE chief scientist, Environemntal Management Science Program funded research into remediating the TAN aquifer using microbes, and what controls microorganisms that are degrading contaminants inthe aquifer. [see Project #55416]

Publication Type: Presentation

Colwell, F. S. (1999). Chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone. Poster presentation at the Berkeley Dynamics of Fluids and Fractured Rock Conference. Berkeley, CA.

Colwell, F. S., Tobin, K., & Wilson, M. (1999, Jan. 7). Control of biologically active degradation zones by vertical heterogeneity: Applications in fractured media. Idaho Water Resources Research Institute (IWRRI) meeting.

Project: 59786

Title: Design and Construction of Deinococcus radiodurans for Biodegradation of Organic Toxins at Radioactive DOE Waste Sites

PI: Dr. Michael J. Daly *Institution:* Uniformed Services Univ. of the Health Sciences

Publication Type: Journal

Lange, C., Wackett, L., Minton, K. & Daly, M. J. (1998). Engineering a recombinant Deinococcus radiodurans for organopollutant degradation in radioactive mixed waste environments. Nature Biotech., 16,929-933.

Project: 59827

Title: The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass

PI: Dr. Michael C. Weinberg *Institution:* University of Arizona

Publication Type: Paper

Jeoung, J. S., Poisl, W. H., Weinberg, M. C., Smith, G. L., & Li, H. (1999). Effect of iron oxidation state on immiscibility temperature in sodium silicate glass. Amer. Ceram. Soc. Bull. 78(4), 205.

Project: 59828

Title: Bioavailability of Organic Solvents in Soils: Input into Biologically Based Dose-Response Models for Human Risk Assessments

PI: Dr. Ronald C. Wester *Institution:* University of California at San Francisco

Publication Type: Journal

Poet, T. S., Corley, R. A , Thrall, K. D., & Wester, R. C. (1999). Assessing the dermal bioavailability of volatile organics in rats. The Toxicologist, 48,339.

Poet, T. S., Corley, R. A., Thrall, K. D., Edwards, J. A., & Wester, R. C. (2000). Exhaled breath analysis and PBPK modeling of the dermal absorption of trichloroethylene in rats. The Toxicologist, 54,147.

Poet, T. S., et. al. (2000, in press). Assessment of the percutaneous adsorption of trichloroethylene in rats and humans using MS/MS real time breath analysis and physiological based pharmacokinetic modeling. Toxicological Sciences.

Poet, T. S., et. al. (2000, in press). Bioavailability of organic solvents in soils: Input into biologically based dose-response models for human-risk assessment. Proceedings of the 15th Annual International Conference on Contaminated Soils and Water.

Poet,T. S., et. al. (2000, in press). Utility of real time breath analysis and physiologically based pharmacokinetic modeling to determine the percutaneous absorption of methyl chloroform in rats andhumans. Toxicological Sciences.

Thrall, K., et. al. (2000, in press). A real-time in vivo method for studying the percutaneous adsorption of volatile chemicals. International Journal of Occupational and Environmental Health.

Wester, R. C., et. al. (1999). An innovative method to detemrine dermal uptake of solvents from soil and water in vivo in humans. The Toxicologist, 48,338.

Wester, R. C., et. al. (2000). Human dermal absorption of trichloroethylene from soil and water. The Toxicologist, 54,148.

Publication Type: Other

Thrall, K. D., Poet, T. S., & Corley, R. A. (1998). An innovative method to determine percutaneous absorption: Real time breath analysis and physiologically based pharmacokinetic modeling. In Bronaugh, R. & Maibach, H. (Eds.), Percutaneous Absorption, Third Edition, Marcel Dekker, Inc. New York, NY.

Publication Type: Presentation

Wester, R. C. (1998). Chemical manufactures association workshop of research planning. Research Triangle Park, NC.

Wester, R. C. (1998, Sept.). Dermal bioavailability. Presetation at NIOSH, Morgantown, WV.

Wester, R. C. (1999). An innovative method to determine dermal uptake of solvents from soil and water. Presentation at the Faculty and Student Undergraduate Research Education Conference. Argonne National Laboratory.

Wester, R. C. (1999). An innovative method to determine dermal uptake of solvents from soil and water in vivo in humans. Presentation at the 15th Annual International Conference on Contaminated Soils and Water. Amherst, MA.

Project: 59849

Title: Radionuclide Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment

PI: Dr. Rodney C. Ewing *Institution:* University of Michigan

Publication Type: Journal

Casas, I., et. al. (1998). The role of pe, pH, and carbonate on the solubility of UO2 and uraninite under nominally reducing conditions. Geochimica et Cosmochimica Acta, 62(13), 2223-2231.

Chen, F. & Ewing, R. C. (1999, in press). Structural contributions to the third-law entropies of uranyl phases. Geochimica et Cosmochimica Acta.

Chen, F., Burns, P. C., & Ewing, R. C. (1999). 79-Se: Geochemical and crystallo-chemical retardation mechanisms. Journal of Nuclear Materials, 275, 81-94.

Chen, F., Burns, P. C., & Ewing, R. C. (1999, in press). Near-field behavior of 99-Tc during the oxidative alteration of spent nuclear fuel. Journal of Nuclear Materials.

Chen, F., Ewing, R. C., & Clark, S. B. (1999). The Gibbs free energies and enthalpies of formation of uranium (VI) phases: An empirical method of prediction. American Mineralogist 84(4),650-654.

Clark, S. B., Ewing, R. C., & Schaumloffel, J. C. (1998). A method to predict free energies of formation of mineral phases in the U(VI)-SiO2-H2O system. Journal of Alloys and Compunds, 271, 189-193.

Ewing, R. C. (1999). Less geology in the geological disposal of nuclear waste. Science, 286, 415-416.

Ewing, R. C., Tierney, M. S., Konikow, L. F., & Rechard, R. P. (1999). Performance assessments of nuclear waste repositories: A dialogue on their value and limitaions. Risk Analysis, 19(5) 933-958.

Fayek, M., Burns, P., Guo, Y. -X., & Ewing, R. C. (2000). Micro-structures associated with uraninite alteration. Journal of Nuclear Materials, 277, 204-210.

Finch, R. J., Cooper, M. A., Hawthorne, F. C., & Ewing, R. C. (1999). Refinement of the crystal structure of rutherfordine. Canadian Mineralogist, 37, 929-938.

Finch, R. J., Hawthorne, F. C., & Ewing, R. C. (1998). Structural relations among schoepite, metaschoepite, and “dehydrated schopite.” Canadian Mineralogist, 36, 831-845.

Jensen, K. A. & Ewing, R. C. (1999, in press). The Okelobondo natural fission reactor, southeast Gabon: Geology, mineralogy, and retardation of nuclear reaction products. Geological Society of America Bulletin.

Zhao, D. & Ewing, R. C. (2000, in press). Alteration products of uraninite from the Colorado Pleateau. Radiochimica Acta.

Publication Type: Presentation

Ewing, R. C. (1999, Sept. 26 - Oct. 1). Results of uranyl phase analyses. Presented at the Seventh International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere. Lake Tahoe, CA.

Publication Type: Proceeding

Chen, F. & Ewing, R. C. (1999). 79-Se: Geochemical and crystallo-chemical retardation mechanisms. Symposium Proceedings of the Materials Research Society, 556, 1115-1122.

Chen, F. & Ewing, R. C. (1999). Structural contributions to the third-law entropy of uranyl phases. Symposium Proceedings of the Materials Research Society, 556, 1017-1024.

Ewing, R. C. (1999). Nuclear waste forms for actinides. Proceedings of the National Academy of Sciences, 96(7), 3432-3439.

Project: 59882

Title: Measurements of Radon, Thoron, Isotopic Uranium and Thorium to Determine Occupational & Environmental Exposure & Risk at Fernald Feed Materials Production Center.
PI: Dr. Naomi H. Harley
Institution: New York University Medical School

Publication Type: Presentation

Harley, N. H. (1999, Jun.). Field results of personal radon and thoron monitor. Annual Health Physics Meeting. Philadelphia, PA. Health Physics 76,163.

Harley, N. H. (1999, Jun.). Results of particle size sampler field tests. Annual Health Physics Meeting. Philadelphia, PA. Health Physics 76,163.

A particle size analyzer that is used for size distribution measurements of inhaled radionuclides particles. Particle size is the major determinant of bronchial doses of radionuclides. [see Project #59882]

Project: 59918

Title: Improved Radiation Dosimetry/Risk Estimates to Facilitate Environmental Management of Plutonium Contaminated Sites
PI: Dr. Bobby R. Scott *Institution:* Lovelace Biomedical & Environmental Research Institute

Publication Type: Journal

Cheng, Y. -S., Zhou, Y., & Chen, B. T. (1999, in press). Particle deposition in a cast of human oral airways. Aerosol Science & Technology.

Hoover, M. D., & Newton, G. J. (1998). Performance testing of continuous air monitors for alpha-emitting radionuclides. Radiat. Prot. Dosim., 79(1-4),499-504.

Hoover, M. D., et. al. (1998). Characterization of enriched uranium dioxide particles from a uranium handling facility. Radiat. Prot. Dos., 79(1-4),57-62.

Hoover, M. D., Mewhinney, C. J., & Newton, G. J. (1999). Modular glovebox connector and associated good practices for control of radioactive and chemically toxic materials. Health Phys., 76(1),66-72.

Osovets, S. V. & Scott, B. R. (1998, Mar. 6). Nonmonotonous character of dose-response relationships. Viniti No. ¼, 645, B98 (in Russian).

Scott, B. R. & Fencl, A. (1999, in press). Variability in PuO2 intake by inhalation: Implications for DOE worker protection. Radiat. Prot. Dosim.

Scott, B. R. (1999). Evaluating the risk of death via the Hematopoietic syndrome mode from prolonged exposure of nuclear workers to radiation delivered at very low raters. Health Physics 74,545-553.

Scott, B. R. (1999). Transformation of C3H 10T1/2 cells. Letter to Editor, J. Radiol. Prot. 19(2),177-179.

Scott, B. R. (1999). Variability in PuO2 intake by inhalation: Implications for worker protection at the U.S. Department of Energy. Radiation Protection Dosimetry. 83(3),221-232.

Scott, B. R., Lyzlov, A. F., & Osovets, S. V. (1998). Evaluating the risk of death via the hematopoietic syndrome mode for prolonged exposure of nuclear workers to radiation delivered at very low rates. Health Physics 74 (5),545-553.

Publication Type: Other

Glissmeyer, J. A., et. al. (1999). American national standard for sampling and monitoring releases of airborne radioactive substances from the stacks and ducts of nuclear facilities. ANSI/HPS N13.1-1999, Health Physics Society, McLean, VA.

Guilmette, R. A. & Scott, B. R. (1998.) Radiation toxicology. In Wexler, P. (Ed.), Encyclopedia of Toxicology, 3,5-18. Academic Press. San Diego, CA.

Publication Type: Poster

Scott, B. R., Hoover, M. D., Neft, R. E., & Fencl, A. F. (1999, Aug. 22-26). Recommendations for improving the interim radionuclide soil action levels for the Rocky Flats Cleanup Agreement. Poster presentation at the 218th American Chemical Society National Meeting. New Orleans, LA.

Publication Type: Presentation

Cheng, Y. -S., Yeh, H. C., Smith, S. M., Cheng, K. H., & Swift, D. L. (1998, Sept. 14-18). Deposition of ultrafine particles in the nasal and tracheobronchial airways. 1998 International Aerosol Conference. Edinburgh, UK.

Hoover, M. D. (1998, Apr. 24). Workplace air sampling methods and good practices. Technical Workshop on Air Sampling: The Big Picture. Savannah River Chapter, Health Physics Society. Aiken, SC.

Hoover, M. D. (1998, Jul. 12). Statistical considerations for aerosol sampling, professional enrichment short course. 43rd Annual Meeting of the Health Physics Society. Minneapolis, MN.

Hoover, M. D. (1999, Jan. 24). Statistical considerations for aerosol sampling. Professional Enrichment Short Course. 32nd Midyear Meeting of the Health Physics Society. Albuquerque, NM.

Hoover, M. D., Newton, G. J., & Cox, F. M. (1998, Feb. 7). Sampling radioactive aerosols. American Academy of Health Physics Short Course. 31st Midyear Meeting of the Health Physics Society. Mobile, AL.

Hoover, M. D., Newton, G. J., & Cox, F. M. (1998, Jul. 15). Flow measurements with rotameters and appropriate corrections. 43rd Annual Meeting of the Health Physics Society. Minneapolis, MN.

Scott, B. R. (1998, Aug.). Improved radiation dosimetry/risk estimates to facilitate environmental management of plutonium contaminated sites. Presentation at the American Chemical Society. New Orleans, LA.

Scott, B. R., et. al. (1998, Jul. 27-30). Evaluating the intake via inhalation of plutonium oxides for the stochastic exposure paradigm. Poster 13 presented at the Environmental Management Science Program Workshop. Chicago, IL.

Smith, S. M., Cheng, Y. S., & Yeh, H. C. (1998, Sept. 14-18). Diffusional deposition of ultrafine particles in human tracheobronchial airways. 1998 International Aerosol Conference, Edinburgh, UK.

Zhang, Z., Wang, X., & Cheng, Y. -S. (1998, Sept. 14-18). Flow pattern and aerosol deposition in the human oral airway. 1998 International Aerosol Conference, Edinburgh, UK.

Publication Type: Proceeding

Glissmeyer, J. A., et. al. (1999). American national standard for sampling and monitoring releases of airborne radioactive substances from the stacks and ducts of nuclear facilities. ANSI/HPS N13.1-1999, Health Physics Society. McLean, VA.

Scott, B. R. (1998). Improved radiation dosimetry/risk estimates to facilitate environmental management of plutonium contaminated sites. In Environmental Management Science Program Workshop, U. S. Department of Energy Publication CONF-980736. Washington, D. C. 25-26.

Project: 59925

Title: Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems

PI: Dr. Bernard R. Cooper *Institution:* West Virginia University

Publication Type: Journal

Cooper, B. R., Becker, J. D., Wills, J. M., & Cox, L. (1998). Calculated lattice relaxation in Pu-Ga. Phys. Rev. B 58B,5143.

Cooper, B. R., Becker, J. D., Wills, J. M., & Cox, L. (1998). Calculated lattice relaxation in Pu-Ga alloys. Journal of Alloys and Compounds, 271-273,367.

Cooper, B. R., Vogt, O., Sheng, Q.G., & Lin, Y.L. (1999, May). From heavy fermions to random-localized-site behavior via Anderson localization. Philosophical Magazine B 79, No. 5,683-702.

Publication Type: Other

Cooper, B. R., Turchi, P.E.A., Gonis, A., Kioussis, N., & Price, D. L. (1999). Correlation effects on stability in Pu metal and its alloys. In Gonis, A. & Kioussis, N. (Eds.), Electron Correlations and Materials Properties. Plenum Publishing.

Publication Type: Presentation

Cooper, B. R. & Beiden, S. (1998). Diffusion of plutonium into transition metallic alloys and of transition metal species into plutonium. Eighth Conference on Computational Research on Materials. Lakeview, WV.

Cooper, B. R. & Beiden, S. (1998). Modeling of diffusion of plutonium in other metals and of gaseous species in plutonium-based systems. Environmental Management Science Workshop. Chicago, IL.

Cooper, B. R. & Beiden, S. (1998, Nov.). Modeling of diffusion of plutonium. Workshop on Environmental Management Science: Integration with End User Needs. Savannah River Site. Aiken, SC.

Cooper, B. R. & Beiden, S. (1998, Nov.). Modeling of interdiffusion of plutonium and other metals. Materials Research Society Meeting. Boston, MA.

Cooper, B. R. & Lederman, D. (1998, Nov.). Portable detection and analysis of plutonium content. Workshop on Environmental Management Science: Integration with End User Needs. Savannah River Site. Aiken, SC.

Cooper, B. R. (1998, Jun. 28 - Jul. 3). Synthesis of many-body theory and electronic structure. International Workshop on Electron Correlations and Materials Properties. Heraklion, Crete, Greece.

Cooper, B. R. (1998, May). Treating electronic and magnetic properties of actinide-based materials beyond one-electron dynamics. School of Actinide Physics and Chemistry. Uppsala, Sweden.

Cooper, B. R. (1999, Apr.). Random 5f localization and the fcc transition and depression of melting temperature in plutonium. 29th Journees des Actinides Conference. Luso, Portugal.

Cooper, B. R. (1999, Mar.). Anomalous electronic behavior and relationship to thermostructural behavior of light actinides. American Physical Society Meeting. Atlanta, GA.

Cooper, B. R., Becker, J. D., Wills, J. M. & Cox, L. (1997, Sept.). Structural relaxation in Pu-Ga via full-potential LMTO calculations. Actinides 97. International Conference. Baden-Baden, Germany.

Cooper, B. R., Kioussis, N., Turchi, P. E. A., Gonis, A., & Price, D. L. (1999, Mar.). Electronic structure of alpha and delta plutonium. American Physical Society Meeting. Atlanta, GA.

Cooper, B. R., Sevilla, E. H., & Fernando, G. W. (1999, Mar.). Equilibrium lattice volume of fcc Pu. American Physical Society Meeting. Atlanta, GA.

Project: 59934

Title: Hazardous Gas Production by Alpha Particles in Solid Organic Transuranic Waste Matrices

PI: Dr. Jay A. LaVerne *Institution:* University of Notre Dame

Publication Type: Journal

Chang, Z. & LaVerne, J. A. (1999, in press). Molecular hydrogen production in the radiolysis of high density polyethylene. J. Phys. Chem.

Publication Type: Presentation

LaVerne, J. A. & Chang, Z. (1999, Aug. 23). Hydrogen production in the radiolysis of polyethylene. 218th ACS National Meeting. New Orleans, LA.

Project: 59960

Title: Direct Investigations of the Immobilization of Radionuclides in the Alteration Phases of Spent Nuclear Fuel

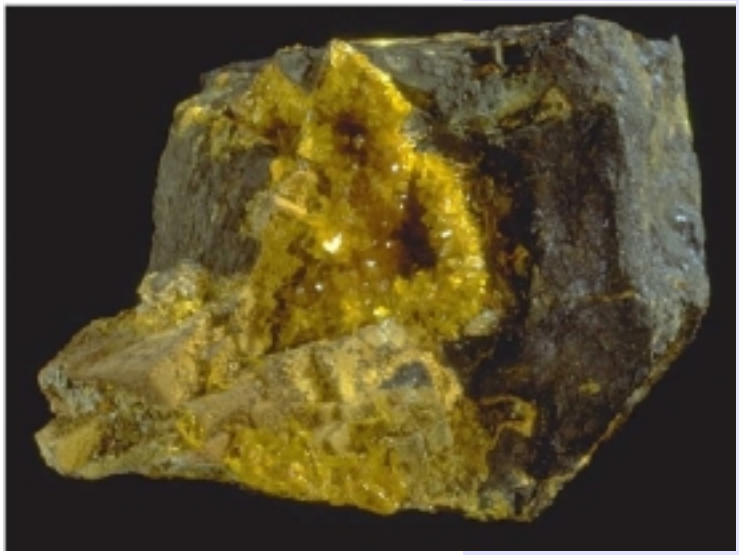
PI: Dr. Peter C. Burns

Institution: University of Notre Dame

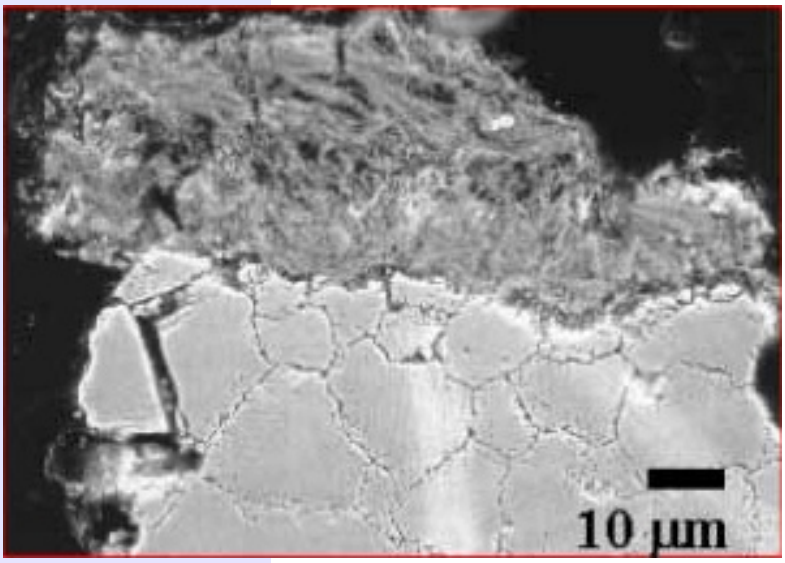
Publication Type: Journal

Burns, P. C. & Finch, R.J. (1999, in press). Wyartite: crystallographic evidence for the first pentavalent-uranium mineral. American Mineralogist.

Burns, P. C. & Hill, F. C. (1998, in press). Implications of the synthesis and structure of the Sr analogue of curite. Canadian Mineralogist.



The mineral uraninite, UO2, is an excellent natural analogue for UO2 (LWR) spent fuel. This photograph shows a specimen of uraninite (black) that has been oxidized under conditions broadly similar to those that will be present in the proposed repository at Yucca Mountain. The uranyl phases that have formed due to the alteration (oxidation) are clearly visible as yellow and orange crystals. We obtain many of the crystals used in our studies from similar natural occurrences. These minerals are typically identical to the phases that form when spent fuel is corroded during laboratory tests at ANL. [see Project #59960]



Laboratory Studies: Argonne National Labs
High Drip Rate Tests:
Alteration Phases:
Boltwoodite: (K,Na)[(UO2)(SiO3OH)](H2O)1.5
Uranophane: Ca[(UO2)(SiO3OH)]2(H2O)5
[see Project #59960]

Burns, P. C. (1998). The structure of boltwoodite and implications of solid-solution towards sodium boltwoodite. Canadian Mineralogist 36,1069-1075.

Burns, P. C. (1998). The structure of compreignacite, K2[(UO2)3O2(OH)3]2(H2O)7. Canadian Mineralogist 36,1061-1067.

Burns, P. C. (1999). Cs boltwoodite obtained by ion exchange from single crystals: Implications for radionuclide release in a nuclear repository. Journal of Nuclear Materials 265,218-223.

Chen, F., Burns, P.C., & Ewing, R.C. (1999, in press). 79 Se: Geochemical and crystallo-chemical retardation mechanisms. Journal of Nuclear Materials.

Hill, F.C. & Burns, P.C. (1999, in press). Structure of a synthetic Cs uranyl oxide hydrate and its relationship to compreignacite. Canadian Mineralogist.

Publication Type: Paper

Burns, P. C. (1999, in press). The crystal chemistry of uranium. Mineralogical Society of America Reviews in Mineralogy.

Publication Type: Presentation

Burns, P. C. & Finch, R. J. (1999). The structure of wyartite: Crystallographic evidence for the first pentavalent-uranium mineral. GAC-MAC. Sudbury, Ontario, Canada.

Burns, P. C. (1998): Topological aspects of uranyl mineral structures. IMA. Toronto, Canada.

Burns, P. C., Finch, R. C. & Wronkiewicz, D. J. (1998). Direct investigations of the immobilization of radionuclides in the alteration products of spent nuclear fuel. DOE Environmental Management Science Program Workshop. Chicago, IL.

Hill, F. C. & Burns, P. C. (1998). Chemical and structural diversity in the uranyl oxide hydrate system. GSA Toronto, Canada.

Hill, F. C. & Burns, P. C. (1998). Investigations of the crystal chemistry of uranyl oxide hydrates. IMA Toronto, Canada.

Hill, F. C. & Burns, P. C. (1999). The importance of uranyl silicates for the disposal of nuclear waste. GAC-MAC. Sudbury, Ontario, Canada.

Kim, C. W. & Wronkiewicz, D. J. (1998). Alteration phases of spent nuclear fuel. Missouri Academy of Sciences, 1998 Annual Meeting.

Publication Type: Proceeding

Chen, F., Burns, P.C., & Ewing, R.C. (1998, in press). 79-Se: Geochemical and crystallo-chemical retardation mechanisms. The Scientific Basis for Nuclear Waste Management XX. MRS Proceedings.

Project: 59967

Title: Aqueous Electrochemical Mechanisms in Actinide Residue Processing
PI: Dr. David E. Morris *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Morris, D. E. (1998, Jul. 27-30). Aqueous electrochemical mechanisms in actinide residue processing. DOE Environmental Management Science Program Workshop. Chicago, IL.

Morris, D. E. (1999, Apr. 21-25). Trends in actinyl electrochemistry: Voltammetry and theory. Presentation at the 217th National Meeting of the American Chemical Society. Anaheim, CA.

Morris, D. E. (1999, Aug. 22-26). Aqueous electrochemical mechanisms in actinide residue processing results. Presentation at the National Meeting of the American Chemical Society. New Orleans, LA.

Morris, D. E. (1999, Aug. 22-26). Aqueous electrochemical mechanisms in mediated dissolution of actinide residues. First Accomplishments of Environmental Management Science Program. National Meeting of the American Chemical Society. New Orleans, LA.

Project: 59977

Title: Synthesis and Characterization of Templated Ion Exchange Resins for the Selective Complexation of Actinide Ions
PI: Dr. George M. Murray *Institution:* Johns Hopkins University Applied Physics Lab

Publication Type: Journal

Bae, S. Y., Southard, G. L., & Murray, G. M., (1999, in press). Molecularly imprinted ion exchange resin for purification, preconcentration and determination of UO2 2+ by spectrophotometry and plasma spectrometry. Analytica Chimica Acta.

Publication Type: Paper

Arnold, B. R., Jenkins, A. L., Uy, O. M., & Murray, G. M. (1999). Progress in the development of molecularly imprinted polymer sensors. JHUAPL Technical Digest, 20,190-198.

Publication Type: Presentation

Kimaro, A. & Murray, G. M. (1998, Mar. 7-12). Synthesis and characterization of templated ion exchange resins for the selective complexation of actinide ions. Abstract No. 2315P, Pittsburgh Conference. Orlando, FL.

Project: 59978

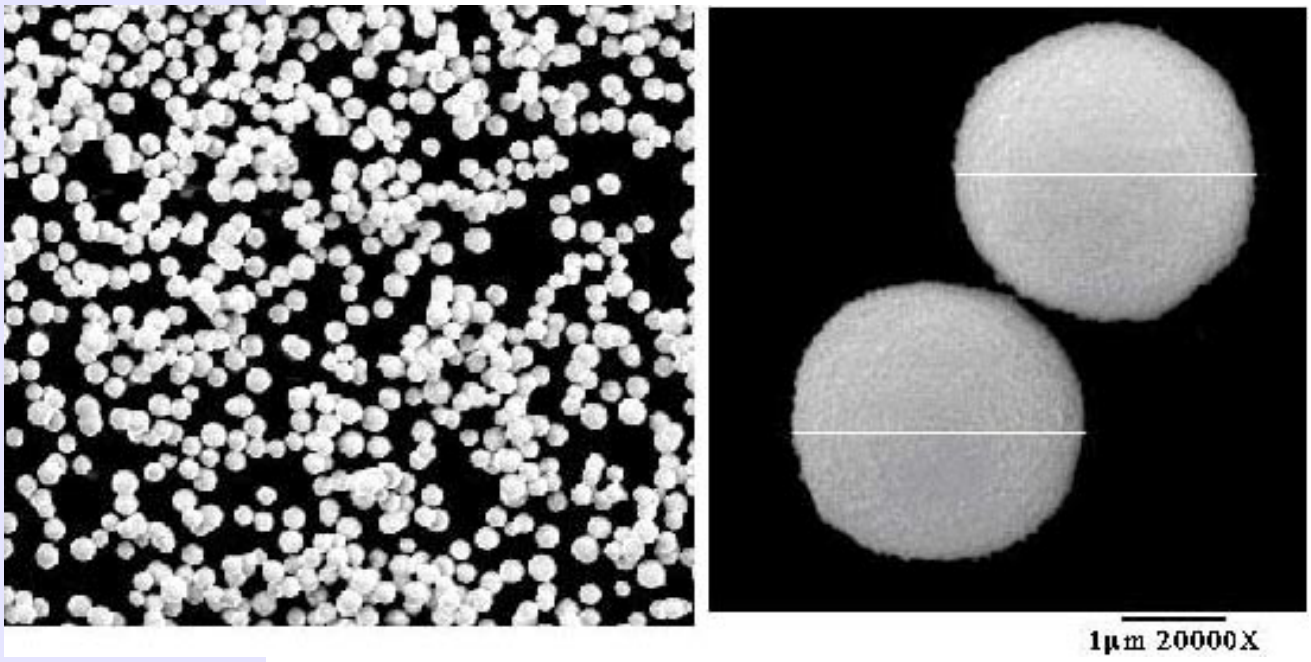
Title: Thermospray Mass Spectrometry Ionization Processes Fundamental Mechanisms for Speciation, Separation and Characterization of Organic Complexants in DOE Wastes

PI: Dr. John E. Caton *Institution:* Oak Ridge National Laboratory

Publication Type: Presentation

Bostick, D. (1999, Aug. 22-26). Separation and speciation of organic complexants in DOE wastes using HPLC on zirconia based stationary phases and thermospray mass spectrometry. Presentation at the National Meeting of the American Chemical Society. New Orleans, LA.

Bostick, D. (1999, Nov. 16). HPLC separation of chelating agents on quaternized polyethyleneimine coated zirconia. Eastern Analytical Symposium. Monchanin, DE.



Electron Micrograph of zirconia particles showing uniform particle size. [see Project #59978]

Caton, J. E. (1998, Jul. 27-30). Thermospray mass spectrometry ionization processes: Fundamental mechanisms for speciation and characterization of organic complexants in DOE wastes. EMSP Workshop, Chicago, IL.

Project: 59981

Title: Real-Time Broad Spectrum Characterization of Hazardous Waste by Membrane Introduction Mass Spectrometry

PI: Dr. Charles W. Wilkerson *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Wilkerson Jr., C. W. (1999, Feb. 22-23). Workshop on harsh environment mass spectrometry. St. Petersburg, FL.

Wilkerson Jr., C. W. (1999, Feb. 28 - Mar. 4). WM99 - HLW, LLW, mixed wastes and environmental restoration - Working towards a cleaner environment. Tucson, AZ.

Wilkerson Jr., C. W. (1999, Mar. 7-12). Pittsburgh conference on analytical chemistry and applied spectroscopy. Orlando, FL.

Project: 59982

Title: Reactivity of Peroxynitrite: Implications for Hanford Waste Management and Remediation

PI: Dr. Sergei V. Lymar *Institution:* Brookhaven National Laboratory

Publication Type: Journal

Coddington, J. W., Hurst, J. K., & Lymar, S. V. (1999). Hydroxyl radical formation during peroxynitrous acid decomposition. J. Am. Chem. Soc., 121,2438-2443.

Coddington, J. W., Wherland, S., & Hurst J. K. (1999). Radical intermediates in peroxynitrite reactions. Nitric Oxide, 3,37.

Czapski, G., Lymar, S. V., & Schwarz, H. A. (1999). Acidity of the carbonate radical. J. Phys. Chem. A, 103,3447-3450.

Gerasimov, O. V. & Lymar, S. V. (1999). Pathways of decomposition and one-electron oxidation by peroxynitrous acid. Nitric Oxide, 3,7.

Goldstein, S., Saha, A., Lymar, S. V., & Czapski, G. (1998). Oxidation of peroxynitrite by inorganic radicals: A pulse radiolysis study. J. Am. Chem. Soc., 120,5549-5554.

Lymar, S. V. & Hurst, J. K. (1998). ACO 2 -catalyzed one-electron oxidations by peroxynitrite: Properties of the reactive intermediate. Inorganic Chemistry, 37,294-301.

Lymar, S. V. & Hurst, J. K. (1998). Radical nature of peroxynitrite reactivity. Chem. Res.Toxicol., 11,714-715.

Project: 59990

Title: Fundamental Chemistry, Characterization, and Separation of Technetium Complexes in Hanford Waste

PI: Dr. Norman C. Schroeder *Institution:* Los Alamos National Laboratory

Publication Type: Other

Schroeder, N. C., Radzinski, S. D., Ashley, K. R., Truong, A. P., & Szczepaniak, P. A. (1998). Technetium oxidation state adjustment for hanford waste processing. In Lombardo, N. J. & Schulz, W. W. (Eds.), Science and Technology for Disposal of Radioactive Tank Waste. Plenum Publishing Corporation. New York, NY.

Publication Type: Proceeding

Ashley, K. R., Whitener, G. D., Schroeder, N. C., Ball, J. R., & Radzinski, S. D. (1999). In Bond, A. H., Dietz, M. L. & Rogers, R. D. (Eds.), Progress in Metal Ion Separation and Preconcentration, ACS Symposium Series 716, American Chemical Society, Washington, D. C. 219.

Project: 59996

Title: Plutonium Speciation, Solubilization, and Migration in Soils

PI: Dr. Mary P. Neu *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Neu, M. P. (1999, Sep. 26-30). The migration behavior of collodial CE, Eu, Zr, and ionic Am and Np in selected solid-matrix materials. Presentation at Migration-99.

Neu, M. P. (1999, Sep. 26-30). Transport behavior of ionic and collodial forms of plutonium. Presentation at Migration-99.

Project: 60017

Title: Removal of Technetium, Carbon Tetrachloride, and Metals from DOE Properties

PI: Dr. Thomas E. Mallouk *Institution:* Pennsylvania State University

Publication Type: Proceeding

Ponder, S. M., Ford, J. R., Darab, J. G., & Mallouk, T. E. (1999, in press). Ferragels: A new family of materials for remediation of aqueous metal ion solutions. MRS Symp. Proceedings.

Project: 60020

Title: Stability of High-Level Waste Forms
PI: Dr. Theodore M. Besmann *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Besmann, T. M., Beahm, E. C., & Spear, K. E. (1999). An approach to thermochemical modeling of nuclear waste glass. In Marra, J. C. & Chandler, G. T. (Eds.), Environmental Issues and Waste Management Technologies IV, 277-87. Ceramic Transactions, 93, American Ceramic Society. Westerville, OH.

Spear, K. E., Besmann, T. M., & Beahm, E. E. (1998). A thermochemical modeling of nuclear waste glass. Hou, P. Y., McNallan, M.J., Oltra, R., Opila, E. J., & Shores, D. A. (Eds.). High Temperature Corrosion and Materials Chemistry. The Electrochemical Society, 10 South Main St. Pennington, NJ. 98-9,512-523.

Spear, K. E., Besmann, T. M., & Beahm, E. E. (1999, Apr.). Thermochemical modeling of glass: Application to high-level nuclear waste glass. MRS Bulletin, 24(4),37-44.

Spear, K. E., Palmisiano, M. N., Pantano, C. G., Besmann, T. M., & Beahm, E. C. (1999). Surface modification of glass by vaporization reactions. Mountziaris, T. J., et. al. (Eds.). Proceeding Symposium Fundamental Gas-Phase and Surface Chemistry of Vapor-Phase Materials Synthesis. The Electrochemical Society, 10 South Main St. Pennington, NJ. 98-23,388-394.

Publication Type: Presentation

Besmann, T. M., Beahm, E. C., & Spear, K. E. (1998, May 6). An approach to thermochemical modeling of high-level nuclear waste glass. 100th annual meeting of the American Ceramic Society. Cincinnati, OH.

Spear, K. E. (1998, 20 May). Thermochemical modeling applied to glass processes in industry and nuclear waste processes. Chemistry Division Seminar, NIST. Gaithersburg, MD.

Spear, K. E. (1998, Nov. 30 - Dec. 4). Thermochemical models of liquid solutions in nuclear waste glass subsystems. Materials Research Society Fall Meeting.

Spear, K. E. (1998, Oct. 15). Thermodynamic and kinetic modeling capabilities. 75 Years of Ceramics at Penn State, and the 53rd annual PCA Forum. Penn State. University Park, PA.

Spear, K. E. (1999, Apr. 25-28). Solid solution thermochemical models for phase systems in high-level nuclear waste glass. 101st annual meeting of the American Ceramic Society.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1998, Jul. 22). Thermodynamic modeling of nuclear waste glass. Gordon Research Conference on High Temperature Materials Chemistry and Diagnostics. Plymouth, NH.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1998, May 7). A thermochemical modeling of nuclear waste glass. Symposium on High Temperature Corrosion and Materials Chemistry. 193rd meeting of the Electrochemical Society. San Diego, CA.

Spear, K. E., Palmisiano, M. N., Pantano, C. G., Besmann, T. M., & Beahm, E. C. (1998, Nov. 6). Surface modification of glass by vaporization reactions. Symposium on the Fundamental Gas-Phase and Surface Chemistry of Vapor-Phase Materials Synthesis. The Electrochemical Society Meeting. Boston, MA.

Project: 60037

Title: Estimation of Potential Population Level Effects of Contaminants on Wildlife
PI: Ms. Linda Mann *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Sample, B. E. & Arenal, C. A. (1999). Allometric models for interspecies extrapolation of wildlife toxicity data. Bull. Environ. Contam. Toxicol., 62,653-663.

Publication Type: Poster

Sample, B. & Arenal, C. (1998, Nov. 15-19). Allometric models for interspecies extrapolation of wildlife toxicity data: Expanding the database. Presentation at the 19th annual SETAC meeting in Charlotte, NC.

Sample, B. E., Arenal, C. A., & Mann, L. K. (1999). Determination of sensitivity of birds and mammals to environmental contamination. Poster presentation at the SETAC annual meeting.

Sample, B., Rose, K., & Suter, II, G. W. (1998, Dec. 1-3). Estimation of potential population-level effects of contaminants on wildlife. Presentation at the Partners in Environmental Technology 98: SERDP Technical Symposium and Workshop. Crystal City, VA.

Sample, B., Rose, K., & Suter, II, G. W. (1998, Jul. 27-30). Estimation of potential population-level effects of contaminants on wildlife. Presentation at the 1st annual meeting of the U. S. Department of Energy Environmental Management Science Program. Chicago, IL.

Publication Type: Presentation

Sample, B. E., Rose, K. A., & Suter II, G. W. (1998, Oct.). Estimation of population-level effects on wildlife based on individual-level exposures: Influence of life history strategies. Proceedings of Symposium on Environmental Contaminants and Terrestrial Vertebrates: Effects on Populations, Communities, and Ecosystems. College Park, MD. 18-21.

Sample, B., Rose, K., & Suter, II, G. W. (1999, Apr.). Estimation of potential population-level effects of contaminants on wildlife. Platform presentation at the NorCal SETAC meeting. Concord, CA.

Sample, B., Rose, K., Suter, II, G. W., & Arenal, C. (1998, Nov. 15-19). Wildlife toxicity data and ecological risk assessment: Problems and solutions. Platform presentation at the 19th annual SETAC meeting. Charlotte, NC.

Project: 60070

Title: The Development of Cavity Ringdown Spectroscopy as a Sensitive Continuous Emission Monitor for Metals

PI: Dr. George P. Miller *Institution:* Mississippi State University

Publication Type: Journal

Miller, G. P. & Winstead, C. B. (1997). Inductively coupled plasma cavity ringdown spectroscopy. J. Anal. Atomic Spectro., 12,907.

Winstead, C. B., Mazzotti, F. J., Mierzwa, J., & Miller, G. P. (1999, in press). Preliminary results for electrothermal atomization - cavity ringdown spectroscopy (ETA-CRDS). Anal. Comm.

Publication Type: Presentation

Miller, G. P. & Winstead, C. B. (1997, Jan. 12-17). ICP-cavity ringdown spectroscopy. Abstract O1-4, Winter Conference in Spectrochemistry. Gent, Belgium.

Miller, G. P. & Winstead, C. B. (1998, Oct. 12-15). ICP-cavity ringdown spectroscopy. Abstract 407, The 25th FACSS Conf. Austin, TX.

Project: 60075

Title: Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations

PI: Dr. J. Thomas Dickinson *Institution:* Washington State University

Publication Type: Paper

Dickinson, J. T. (1998, Aug.). Mechanisms for and characterization of particulate generation by laser irradiation of inorganic crystalline materials. DOE-EMSP Workshop on Waste Characterization. Chicago, IL.

Dickinson, J. T. (1998, Jun.). Ejection of droplets and fracture particles from single crystal NaNO 3 during pulsed laser irradiation. Gordon Research Conference on Laser Interaction with Materials.

Dickinson, J. T. (1999, Jun.). UV laser interactions with inorganic single crystals with molecular anions. American Chemical Society. Portland, OR.

Dickinson, J. T. (1999, Mar.). High energy ions from UV laser irradiation of cleaved ionic crystals. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). Laser desorption of energetic ions from single crystal NaNO 3 at 1064 nm. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). The effect of surface treatment on excimer laser induced positive ion desorption in brushite. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). Ultrafast and nanosecond laser induced desorption from ionic solids. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, May). Laser-induced positive ion and neutral atom/ molecule emission from single crystal CaHPO 4 2H 2 O: The role of radiation induced defects. Materials Research Society. San Francisco, CA.

Dickinson, J. T. (1999, May). Studies of particulate formation by laser ablation in support of chemical analysis of high level mixed waste. American Ceramics Society. Indianapolis, IN.

Hedges, A. L., Mendoza, A., Alexander, M. L., Langford, S.C., & Dickinson, J. T. (1999, Mar.) Investigations of particle formation by laser ablation for elemental analysis. 217th ACS meeting. Anaheim, CA.

Publication Type: Presentation

Alexander, M. L., Langford, S. C., & Dickinson, J. T. (1998, Oct.). Fundamental mechanisms of particulate formation by laser ablation for inductively coupled plasma mass spectrometry (LA/ICP-MS). Presentation at the SPIE East conference. Boston, MA.

Alexander, M. L., Langford, S.C., & Dickinson, J. T. (1999, Mar.). Particle generation by laser ablation in support of chemical analysis of high level mixed waste from plutonium production operations. Invited presentation at the DOE Characterization and Monitoring Sensor Technology (CMST) meeting. Gaithersburg, MD.

Dickinson, J, T. (1999, Jan.). The desorption of energetic ions from ionic crystals. Dept. of Physics, Washington State University. Pullman, WA.

Dickinson, J. T. (1998, Jun.). The laser desorption of ions from ionic crystals. Gordon Conference on Laser Materials Interactions.

Dickinson, J. T. (1998, Nov.). New models of laser desorption and particle formation. Physics Dept. Colloquium. University of Linz, Austria.

Dickinson, J. T. (1998, Oct. - Nov.). Topics in surface dynamics. Guest Lecturer, Institute of Applied Physics. University of Linz, Austria.

Dickinson, J. T. (1998, Oct.). Mechanisms for and characterization of particulate generation by laser irradiation of inorganic crystalline materials. FACS National Meeting. Austin TX.

Dickinson, J. T. (1999, Jan.). The use of lasers in chemical analysis. University of Minho. Braga, Portugal.

Dickinson, J. T. (1999, Jun.). Laser desorption and chemical analysis. Departments of Physics and Chemistry. U. of Heidelberg, Germany.

Dickinson, J. T. (1999, Jun.). The laser desorption of ions from ionic crystals. E-MRS Symposium on Laser Materials Interactions. Strasbourg, France.

Dickinson, J. T. (1999, Jun.). The use of lasers in chemical analysis of toxic materials. Paul Scherrer Institute. Villigen PSI, Switzerland.

Project: 60077

Title: Development of Nuclear Analysis Capabilities for DOE Waste Management Activities

PI: Dr. Cecil V. Parks *Institution:* Oak Ridge National Laboratory

Publication Type: Theses/Dissertations

Rearden, B. T. (1999). Development of SAMS: A three-dimensional sensitivity analysis module for the SCALE code system. PhD dissertation at Texas A&M University.

Project: 60096

Title: Rational Synthesis of Imprinted Organofunctional Sol-Gel Materials for Toxic Metal Separation

PI: Dr. Ziling Benjamin Xue *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

Dai, S., et. al. (1999). Imprint coating: Novel synthesis of selective functionalized ordered mesoporous sorbents. Angew. Chem. Int. Ed., 38,1235-1239.

Dai, S., et. al. (1999, in press). A new methodology to functionalize surfaces of ordered mesoporous materials based on ion exchange reactions. Adv. Mater.

Shin, Y. S., Burleigh, M. C., Dai, S., Barnes, C. E., & Xue, Z. L. (1999). Investigation of uranyl adsorption on mesoporous titanium-based sorbents. Radiochim. Acta. 84,37-42.

Project: 60115

Title: Advanced High Resolution Seismic Imaging, Material Properties Estimation and Full Wavefield Inversion for the Shallow Subsurface

PI: Dr. Alan Levander *Institution:* Rice University

Publication Type: Journal

Zelt, C. A., Hojka, A. M., Flueh, E. R., & McIntosh, K. D. (1999, in press). 3D simultaneous seismic refraction and reflection tomography of wide-angledata from the central Chilean margin. Geophys. Res. Lett.

Zelt, C. A., Optimal utilization of sub-optimal 3D wide-angle data. Seis. Res. Lett., 70,255.

Publication Type: Presentation

Akerberg, P., Dana, D., Levander, A., Zelt, C., & Henstock, T. (1998). High resolution shallow seismic imaging at an open pit copper mine. 10th Annual IRIS Workshop. Santa Cruz, CA.

Dana, D., Akerberg, P., Levander, A., Zelt, C., & Henstock, T. J. (1998). Shallow-seismic investigation at an open pit copper mine: A comparison with drill data. EOS, Trans. Am. Geophys. Union, 79,F652.

Dana, D., Akerberg, P., Zelt, C., Levander, A., & Henstock, T. (1998). High resolution seismic imaging at a porphyry copper mine. Society of Exploration Geophysicists. New Orleans, LA.

Dana, D., Zelt, C., & Levander, A. (1999). High-resolution seismic survey over a near-surface contamination site. SEG International Exposition and Sixty-Ninth Annual Meeting.

Passmore, P., Keller, G. R., Miller, K. C., Levander, A., & McMechan, G. (1999). Single-channel recorder test results from two different active source experiments. Seism. Res. Letters, 70,243.

Zelt, C. A. & Hojka, A. M. (1998). 3D simultaneous seismic refraction and reflection tomography of wide-angle traveltime data from the central Chilean margin. EOS, 79,F638.

Project: 60118

Title: Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms
PI: Dr. Mark A. Williamson
Institution: Argonne National Laboratory

High temperature solution calorimeter at Los Alamos National Laboratory. This calorimeter is the same type used in studies of non-radioactive materials but has been installed in a section of the laboratory to allow the use of Pu-bearing samples to measure the formation energetics of Pu-bearing materials. A 1997 DOE EMSP grant helped establish the facility and will support the measurement of Pu-bearing waste ceramics being synthesized at LLNL. [see Project #60118]

Publication Type: Journal

"Thermodynamics of Formation for Two Cerium Aluminum Oxides, CeAlO3(s) and CeAl12O19.918(s), and Cerium Sesquioxide, Ce2O3(s) at T = 298.15 K", R. L. Putnam, A. Navrotsky, E. H. P. Cordfunke, and M. E. Huntelaar, J. Chem. Thermo. (submitted)

Putnam, R. L., Navrotsky, A., Cordfunke, E. H. P., & Huntelaar, M. E. (1999, in press). Thermodynamics of formation for two cerium aluminum oxides, CeAlO3 and CeAl12O19.918, and cerium sesquioxide, Ce2O3 at T= 298.15 K. J. Chem. Thermodynamics.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., & Boerio-Goates, J. (1999). Heat capacity, third law entropy, and formation energetics of zirconolite, CaZrTi2O7. Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries IV, Ceramic Transactions, 93,339.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., Boerio-Goates, J., & Shapiro, J. L. (1999). Thermodynamics of formation of zirconolite (CaZrTi2O7) from T = 298.15 K to T = 1500 K. J. Chem. Thermo. 31(3),229-243.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., Shapiro, J. L., & Boerio-Goates, J. (1999). Heat capacity, third law entropy, and formation energetics of zirconolite, CaZrTi2O7. In Marra, J. C. & Chandler, G. T. (Eds.), Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries IV, Ceramic Transactions, 93. The American Ceramic Society. Westerville, OH.

Woodfield, B. F., Boerio-Goates, J., Shapiro, J. L., Putnam, R. L., & Navrotsky, A. (1999). Molar heat capacity and thermodynamic functions of zirconolite, CaZrTi2O7. J. Chem. Thermodynamics 31(3),245-253.

Publication Type: Other

Putnam, R. L., Ph.D. Dissertation. (1999, Nov.). Department of Geosciences, Princeton University, NJ.

Publication Type: Presentation

Putnam, R. L., et. al., (1998, Dec.). Thermochemistry of Hf-zirconolite, CaHfTi2O7. Scientific Basis for Nuclear Waste Management, Materials Research Society.

Publication Type: Proceeding

Putnam, R. L., et. al. (1999, in press). Thermochemistry of Hf-zirconolite, CaHfTi2O7. MRS Proceedings.

Project: 60123

Title: Potential-Modulated Intercalation of Alkali Cations into Metal Hexacyanoferrate Coated
PI: Dr. Daniel T. Schwartz *Institution:* University of Washington

Publication Type: Journal

Haight, S. M., Schwartz, D. T., & Lilga, M. A. (1999). In-situ oxidation state profiling of nickel hexacyanoferrate derivatized electrodes using line-imaging Raman spectroscopy and multivariate calibration. J. Electrochem. Soc. 146,1866.

Project: 60144

Title: Flow Visualization of Forced and Natural Convection in Internal Cavities
PI: Dr. John C. Crepeau *Institution:* University of Idaho

Publication Type: Journal

Condie, K. G., Stoots, C. M., McEligot, D. M., Becker, S., & Durst, F. (1998). Measurements of induced boundary layer transition in the new INEEL Matched-Index-of-Refraction flow system. American Physical Society Fluid Dynamics Meeting. Bulletin APS. 43,2092.

Nishimura, M., Fujii, S., Shehata, A. M., Kunugi, T., & McEligot, D. M. (1997). Prediction of forced gas flows in circular tubes at high heat fluxes. NuReTH-8, Kyoto.

Shehata, A. M. & McEligot, D. M. (1998). Mean structure in the viscous layer of stongly-heated internal gas flows. International Journal of Heat Mass Transfer. 41,4297-4313.

Publication Type: Presentation

Ezato, K., Shehata, A. M., Kunugi, T., & McEligot, D. M. (1997). Numerical predictions of transitional features of turbulent forced gas flows in circular tubes with strong heating. ASME Fluids Engineering Conference. Vancouver, British Columbia, Canada.

McEligot, D. M. (1997). Maximum allowable heat flux for a submerged tube bundle. Engineering Conference on Convective Flow and Pool Boiling. Irsee, Germany.

McEligot, D. M., Shehata, A. M., & Kunugi, T. (1998). Prediction of strongly-heated gas flows. Invited presentation at the Engineering Foundation Conference on Turbulent Heat Transfer II, I,33-47. Manchester, U. K.

Publication Type: Proceeding

Crepeau, J. C., et. al. (1998, Sept.). Fluid mechanic studies relating to drying and passivation in an idealized SNF cannister. ANS 3rd Topical Meeting on Spent Nuclear Fuel and Fissile Material Management. Charleston, SC.

McCreery, G. E. & Martineau, R. M. (1998, Nov.). An experimental investigation of steam injection in fractured porous media. ASME International Mechanical Engineering Congress. Anaheim, CA.

McCreery, G. E., et. al. (1999, Sept. 6-9). Flow visualization and velocity measurements in a model fuel storage canister. ANS Global '99 International Conference on Future Nuclear Systems. Jackson, WY.

McCreery, G. E., Kullberg, C. M., Schultz, R. R., Yonomoto, T., & Anoda, Y. (1997). Heat transfer modeling of the LSTF Passive Residual Heat Removal System. ASME Nuclear Engineering Division, ASME Symposium of the 1997 International Mechanical Engineering Congress. Dallas, TX., 97-106.

Project: 60150

Title: Genetic Engineering of a Radiation-Resistant Bacterium for Biodegradation of Mixed Wastes

PI: Dr. Mary E. Lidstrom *Institution:* University of Washington

Publication Type: Poster

Meima, R., Rothfuss, H., Gewin, L., & Lidstrom, M. E. (1998, Jul. 27-30). Genetic engineering of a radiation-resistant bacterium for biodegradation of mixed wastes. Poster presentation at the DOE Environmental Management Science Program Workshop. Chicago, IL.

Project: 60155

Title: Measurements and Models for Hazardous Chemical and Mixed Wastes

PI: Dr. Cynthia Holcomb *Institution:* National Institute of Standards & Technology - Boulder

Publication Type: Journal

Mathias, P. M., Naheiri, T., & Oh, E. M. (1989). A density correction for the Peng-Robinson equation of state. Fluid Phase Equilibria, 47,77-87.

Project: 60158

Title: Development of Radon-222 as a Natural Tracer for Monitoring the Remediation of NAPL Contamination in the Subsurface

PI: Dr. Lewis Semprini *Institution:* Oregon State University

Publication Type: Other

Semprini, L., Cantaloub, M., Gottipati, S., Hopkins, O., & Istok, J. (1998). Radon-222 as a natural tracer for quantifying and monitoring NAPL remediation. In Wickramanayake, G. B. & Hinchee, R. E. (Eds.), Nonaqueous-phase Liquids: Remediation of Chlorinated and Recalcitrant Compounds. Battelle Press, Columbus, OH. 137-142.

Publication Type: Presentation

Cantaloub, M. (1998, Nov. 16-19). The role of cocktail solvent on radon measurement by liquid scintillation analysis. Packard Instrument Co. Environmental LSC Workshop at the 44th Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry. Albuquerque, NM.

Cantaloub, M., Higginbotham, J., Istok, J. & Semprini, L. (1998, Nov. 16-19). Interaction of sample, cocktail and headspace volume when measuring aqueous Rn in small volume samples. 44th Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry. Albuquerque, NM.

Cantaloub, M., Humphrey, M., Istok, J., & Semprini, L. (1998, Dec. 6-10). Monitoring NAPL remediation using Rn-222 as an in-situ indicator. 1998 Fall Meeting of the American Geophysical Union. San Francisco, CA.

Cantaloub, M., Istok, J., & Semprini, L. (1998, Dec. 1-3). Radon-222 as a natural tracer for monitoring the remediation of NAPL contamination in the subsurface. Strategic Environmental Research and Development Program (SERDP) and Environmental Security Technology Certification Program (ESTCP) Technical Symposium and Workshop. Arlington, VA.

Cantaloub, M., Istok, J., & Semprini, L. (1998, Jul. 20-23). Investigations of Radon-222 as an internal tracer for monitoring NAPL remediation. Symposium on Environmental Models and Experiments Envisioning Tomorrow; Behavior and Remediation of Nonaqueous Phase Liquid Contaminants in the Subsurface. UC Irvine, CA.

Cantaloub, M., Istok, J., & Semprini, L. (1998, Oct. 20-23). Site assessment and remediation monitoring using naturally occuring Rn-222. The 5th International Petroleum Environmental Conference. Albuquerque, NM.

Semprini, L., Istok, J., & Cantaloub, M. (1998, Jul. 27-30). Development of Rn-222 as a tracer for monitoring the remediation of NAPL contamination in the subsurface. Department of Energy Environmental Management Science Program Scientific Workshop, Rosemont, IL.

Project: 60162

Title: Enhancements to & Characterization of the Very Early Time Electromagnetic (VETEM) Prototype Instrument & Applications to Shallow Subsurface Imaging at Sites in the DOE Complex

PI: Dr. David L. Wright *Institution:* U.S. Geological Survey - Denver

Publication Type: Journal

Cui, T. J. & Chew, W. C. (1999, in press). Modeling of arbitrary wire antennas above ground. IEEE Trans. on Geoscience and Remote Sensing.

Cui, T. J. & Chew, W. C. (1999, Jun.). Fast algorithm for electromagnetic scattering by buried conducting plates of large size. IEEE Trans. on Antennas and Propagation, 47(6),1116-1118.

Cui, T. J. & Chew, W. C. (1999, Mar.). Fast evaluation of sommerfeld integrals for EM scattering and radiation by three-dimensional buried objects. IEEE Trans. on Geoscience and Remote Sensing, GE-37(2),887-900.

Cui, T. J. & Chew, W. C. (1999, Sept.). Fast algorithm for electromagnetic scattering by buried 3D dielectric objects of large size. IEEE Trans. on Geoscience and Remote Sensing, GE-37(5),2597-2608.

Publication Type: Paper

Cui, T. J. & Chew, W. C. (1999, Aug. 15-22). Fast algorithm for electromagnetic scattering by buried 3D dielectric objects of large size. XXVIth General Assembly of the International Union of Radio science, 982. Toronto, Canada.

Cui, T. J. & Chew, W. C. (1999, Jul. 12-15). Accurate model of arbitrary wire antennas in free space, above or inside ground. Digest of IEEE Antennas and Propagation Society International Symposium, 2, 982-985. Orlando, FL.

Wright, D. L. et. al. (1999, Aug. 13-21). An assessment of the prototype very early time electromagnetic system (VETEM). XXVIth General Assembly of the International Union of Radio science. Toronto, Canada.

Wright, D. L., et. al. (1999, Mar. 14-18). New field and modeling results from a simulated waste pit using the enhanced very early time electromagnetic (VETEM) prototype system. Proceeding of the 12th Annual Symposium on the Applications of Geophysics to Environmental and Engineering Problem (SAGEEP), Oakland, CA.

Publication Type: Report

Cui, T. J. & Chew, W. C. (1999, Aug.). Novel difraction tomographic algorithm for imaging two-dimensional dielectric objects buried under a lossy earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-21-99. Also submitted to IEEE Trans. on Geoscience and Remote Sensing.

Cui, T. J. & Chew, W. C. (1999, Jan.). Accurate model of arbitrary wire antennas in free space, above or inside ground. Electromagnetics Laboratory, University of Illinois at Urbana-Champaign, Research Report No. CCEM-2-99. Also submitted to IEEE Trans. on Antennas and Propagation.

Cui, T. J. & Chew, W. C. (1999, Jul.). Frequency-spatial domain inverse scattering of two-dimensional dielectric objects buried under a lossy earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-19-99. Also submitted to IEEE Trans. on Microwave Theory and Techniques.

Cui, T. J., et. al. (1999, Mar.). Numerical modeling of an enhanced very early time electromagnetic (VETEM) prototype system. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-7-99. Also submitted to IEEE Antennas and Propagation Magazine.

(a)

(b)

Automatic geophone-planting device. (a) Folded plow, ready for transport. Channel iron welded to V-shaped blades can be seen at top right. (b) Plow ready for automatic geophone planting. Channel iron with geophones attached can be seen in the foreground as a white line running from left to right. [see Project #60199]

Cui, T. J., et. al. (1999, May). Nonlinear inverse scattering of two-dimensional dielectric objects buried under a lossy earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-12-99. Also submitted to IEEE Trans. on Geoscience and Remote Sensing.

Project: 60163

Title: Investigation of Techniques to Improve Continuous Air Monitors Under Conditions of High Dust Loading in Environmental Settings

PI: Dr. Stephen D. Schery

Institution: New Mexico Institute of Mining & Technology

Publication Type: Presentation

Rodgers, J. C., Wasiolek, P. T., Schery, S. D., & Alcantara, R. E. (1998, Nov. 1-6). High resolution real-time optical studies of radiological air sample processes in an environmental continuous air monitor. 1998 SPIA Symposium on Industrial and Environmental Monitors and Biosensors. Boston, MA. LA-UR-98-1684.

Project: 60199

Title: Seismic-Reflection and Ground Penetrating Radar for Environmental Site Characterization

PI: Dr. Don W. Steeples

Institution: University of Kansas

(a) (b)

Field Layout. (a) View from one end of the plow. The channel iron with geophones and wiring attached runs from lower right to just above center of photo. (b) Plow with test-line geophones planted in the ground under the rear of the plow. Comparison-line geophones with normal plants are about 75cm to the right of the test line. [see Project #60199]

Publication Type: Journal

Baker, G. S., Schmeissner, C., Steeples, D. W., & Plumb, R. G. (1999). Seismic reflections from depths of less than two meters. Geophys. Res. Lett., 26(2),279-282.

Baker, G. S., Steeples, D. W., & Schmeissner, C. (1999). In-situ, high-frequency P-Wave velocity measurements within 1 m of the Earth's surface. Geophysics, 64(2),323-325.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Pavlovic, M. (2000, in press). On coincident seismic and radar imaging. Geophysics.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Spikes, K. T. (2000, in press). Source-dependent frequency content of ultrashallow seismic reflection data. Bulletin of the Seismological Society of America.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Spikes, K. T. (2000, in press). Ultrashallow seismic reflection monitoring of seasonal fluctuations in the groundwater table. Environmental and Engineering Geoscience Journal.

Steeples, D. W. & Baker, G. S. (1998, Jun.). Near-surface contributions to seismic static corrections. AAPG Explorer, 19, 20-21,29.

Steeples, D. W., Baker, G. S., & Schmeissner, C. (1999). Toward the autojuggie: Planting 72 geophones in 2 seconds, Geophysical Research Letters, 26(8),1085-1088.

Steeples, D. W., Baker, G. S., Schmeissner, C., & Macy, B. K. (1999). Geophones on a board. Geophysics, 64(3),809-814.

Publication Type: Poster

Plumb, R. G., Steeples, D. W., Baker, G. W., Schmeissner, C., & Pavlovic, M. (1999, Jun.). A combined ground-penetrating radar and shallow seismic reflection approach to characterizing hydrological flow. International Geoscience and Remote Sensing Society (IGARSS) meeting. Hamburg, Germany.

Publication Type: Presentation

Baker, G. S., Plumb, R. G., Steeples, D. W., Pavlovic, M., & Schmeissner, C. (1998). Coincident GPR and ultrashallow seismic imaging in the Arkansas River Valley, Great Bend, Kansas. SEG Expanded Abstracts, SEG 1998 International Meeting. New Orleans, LA. 859-861.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Macy, B. K. (1998). In-situ, high-resolution P-wave velocity measurements within 1 m of the Earth's surface. SEG Exp. Abstr., SEG 1998 International Meeting. New Orleans, LA. 856-858.

Steeples, D. W., Baker, G. S., & Schmeissner, C. (1998, Dec. 6-10). Toward the autojuggie: Planting 72 geophones in 2 seconds. (1998). American Geophysical Union, 1998 Fall Meeting. San Francisco, CA.

Steeples, D. W., Baker, G. S., Schmeissner, C., & Macy, B. K. (1998). Geophones on a board. SEG Exp. Abstr., SEG 1998 International Meeting. New Orleans, LA. 852-855.

Publication Type: Theses/Dissertations

Baker, G. S. (1999, May). Seismic imaging shallower than three meters. Ph. D. dissertation. The University of Kansas, Lawrence, KS.

Pavlovic, M. (2000). Ground-penetrating radar in shallow aquifer detection and monitoring. Master's Thesis. University of Kansas. Lawrence, KS.

Project: 60217

Title: Optically-Based Array Sensors for Selective in Situ Analysis of Tank Waste
PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Ji, H. -F., Brown, G. M., & Dabestani, R. (1999). Calix[4]arene-based Cs+ selective optical sensor. Chem. Comm., 609.

Ji, H. -F., Dabestani, R., Brown, G. M., & Hettich, R. L. (1999). Spacer length effect on the photoinduced electron transfer fluorescent probe for alkali metal ions. Photochem. Photobiol. 69,513.

Publication Type: Presentation

Ji, H. -F., Dabestani, R., & Brown, G. M. (1998, Aug.). Fluorescence probes for the detection of potassium ions. Presentation at the American Chemical Society National Meeting. Boston, MA.

Project: 60218

Title: Novel Mass Spectrometry Mutation Screening for Contaminant Impact Analysis

PI: Dr. C. H. Winston Chen *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Chen, C. H., et. al. (1999). Laser desorption mass spectrometry for high throughput DNA analysis and its applications. SPIE Int. Soc. Opt. Eng. 3602,338-345.

Golovlev, V. V., Allman , S. L., Garrett, W. R., Taranenko, N. I., & Chen, C. H. (1997). Laser induced acoustic desorption. International Journal of Mass Spectrometry and Ion Processes, 169/170,69-78.

Isola, N. R., Allman, S. L., Golovlev, V. V., & Chen, C. H. (1999). Chemical cleavage sequencing of DNA using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry. Analytical Chemistry, 71,2266-2269.

Taranenko, N. I., et. al. (1998). Matrix-assisted laser desorption/ionization for short tandem repeat loci. Rapid Comm. Mass Spectrom., 12,413-418.

Taranenko, N. I., et. al. (1998). Sequencing DNA using mass spectrometry for ladder detection. Nucleic Acids Research, 26(10),2488-2490.

Taranenko, N. I., Potter, N. T., Allman, S. L., Golovlev, V. V., & Chen, C. H. (1999). Detection of trinucleotide expansion by matrix-assisted laser desorption/ ionization time-of-flight mass spectrometry. Genetic Analysis, 15,25-31.

Publication Type: Presentation

Chen, C. H. (1999, Mar. 26). Laser desorption mass spectrometry for rapid nucleic acid analysis. American Physical Society Centennial Meeting.

Project: 60219

Title: Development of Advanced Electrochemical Emission Spectroscopy for Monitoring Corrosion in Simulated DOE Liquid Waste
PI: Dr. Digby D. MacDonald *Institution:* Pennsylvania State University

Publication Type: Presentation

Sikora, E. & Macdonald, D. D. (1999, May 9-15). Passive films on iron formed in the presence of EDTA. Presentation at the 8th International Symposium on Passivity of Metals and Semiconductors. Jasper, Canada.

Project: 60231

Title: Novel Miniature Spectrometer for Remote Chemical Detection
PI: Dr. Andrew C. R. Pipino *Institution:* National Institute of Standards & Technology

Publication Type: Journal

Pipino, A. C. R. (1998, Nov.). Evanescent wave cavity ring-down spectroscopy for ultra-sensitive chemical detection. SPIE 3535,57. Boston, MA.

Pipino, A. C. R., et. al. (1997). Evanescent wave cavity ring-down spectroscopy with a total-internal-reflection minicavity. Rev. Sci. Instrum., 68,2978.

Pipino, A.C.R., et. al. (1997). Evanescent wave cavity ring-down spectroscopy as a probe of surface processes. Chem. Phys. Lett., 280,104.

Publication Type: Patent

Pipino, A. C. R. (1998, Nov. 10). Broad band intra-cavity total reflection chemical sensor. US5835231.

Pipino, A. C. R. (1999, Aug. 24). Intra-cavity total reflection for high sensitivity measurement of optical properties. US5943136.

Pipino, A. C. R. (1999, Nov. 16). Intra-cavity total reflection for high sensitivity measurement of optical properties. US5986768.

Project: 60271

Title: Characterization of a New Family of Metal Transport Proteins
PI: Dr. Mary Lou Guerinot *Institution:* Dartmouth College

Publication Type: Journal

Eng, B. H., Guerinot, M. L., Eide, D., & Saier, M. H. J. (1998). Sequence analyses and phylogenetic characterization of the ZIP family of metal ion transport proteins. J. Membr. Biol., 166,1-7.

Gitan, R. S., Luo, H., Rodgers, J., Broderius, M., & Eide, D. (1998). Zinc-induced inactivation of the yeast ZRT1 zinc transporter occurs through endocytosis and vacuolar degradation. J. Biol. Chem., 273, 28617-28624.

Guerinot, M. L. & Eide, D. (1999). Zeroing in on zinc uptake in yeast and plants. Curr. Opin. Plant Biol., 2, 244-249.

Korshunova, Y. O., Eide, D., Clark, W. G., Guerinot, M. L., & Pakrasi, H. B. (1999). The IRT1 protein from Arabidopsis thaliana is a metal transporter with broad specificity. Plant Mol. Biol., 40,37-44.

Project: 60283

Title: Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation

PI: Dr. Michael J. Pellin *Institution:* Argonne National Laboratory

Publication Type: Poster

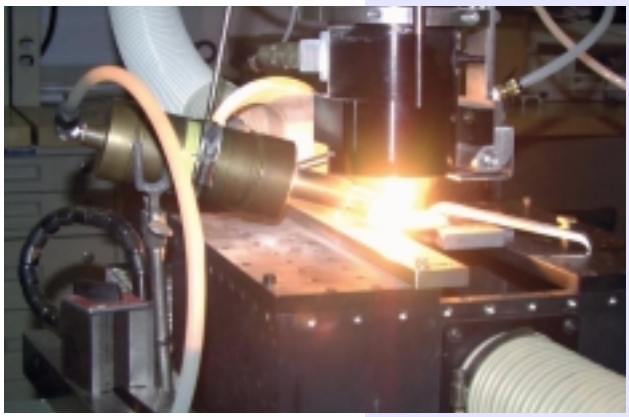
Savina, M. R., Pellin, M. J., Leong, K., & Xu, Z. (1998, Jul.). Waste volume reduction using surface characterization and decontamination by laser ablation. Presentation at EMSP Workshop. Rosemont, IL.

Publication Type: Presentation

Pellin, M. J., Savina, M. R., Reed, C. B., Wang, Y., & Xu, Z. (1999, Mar.). Waste volume reduction using surface characterization and decontamination by laser ablation. Presentation at Characterization, Monitoring, and Sensing Workshop. Gaithersburg, MD.

Publication Type: Proceeding

Savina, M. R., Xu, Z., Wang, Y., Leong, K., & Pellin, M. J. (1998). Laser ablation of concrete. Proceedings of the 17th International Conference on Applications of Lasers and Electro-Optics, 85A,219-226.



Laser Ablation System – 1.6 kw pulsed Nd:YAG laser system with fiber optic beam delivery. Advantages of this system over conventional scabbling are for hard-to-reach places and remote decontamination. [see Project #60283]

Project: 60296

Title: Research Program to Investigate the Fundamental Chemistry of Technetium

PI: Dr. Norman M. Edelstein *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Presentation

Edelstein, N. M. (1999, Sept. 22-25). Technetium chemistry in highly basic solutions. Presentation at the Technetium Chemistry Workshop. Hanford, WA.

Project: 60313

Title: Radiation Effects on Transport and Bubble Formation in Silicate Glasses
PI: Dr. Alexander D. Trifunac *Institution:* Argonne National Laboratory

Publication Type: Journal

Shkrob, I. A., Tadjikov, B. M., Chemerisov, S. D. & Trifunac, A. D. (1999). Electron trapping and hydrogen atoms in oxide glasses. J. Chem. Phys., 111,5124-5140.

Project: 60328

Title: High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts
PI: Dr. Ki-Ha Lee *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Report

Frangos, W. & Becker, A. (1998). Magnetic fields of AM band radio broadcast signals at the Richmond Field Station. Lawrence Berkeley National Lab Report LBNL-42654.

Lee, K. H. (1997). High-frequency electric field measurement using a toroidal antenna. Lawrence Berkeley National Lab Report LBNL-39894, UC-2040.

Project: 60345

Title: New Silicotitanate Waste Forms: Development and Characterization
PI: Dr. Mari Lou Balmer *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Nyman M., et. al. (1999, in press). Synthesis and characterization of a new microporous Cs-Ti-Si-O-H2O ion exchanger. Chemistry of Materials.

Nyman, M., et. al. (1999, in press). Synthesis and characterization of Cs2TiSi4O11: A novel durable phase with potential waste form applications. Chemistry of Materials.

Publication Type: Patent

Balmer, M. L. (2000, Jan. 14). Novel niobate based molecular sieves. Pending.

Publication Type: Presentation

Balmer, M. L. (1999). Results on phases a, b (Si, Ti phases) and e, f (Niobate phases). United Engineering Foundations: Metals Separations for 2000 and beyond.

Balmer, M. L., et. al. (1999, Apr. 25-28). Ceramic wasteforms from Cs-loaded crystalline silicotitanates. 101th Annual Meeting of the American Ceramic Society. Indianapolis, IN.

Nyman, M. D. & Nenoff, T. M. (1999, Jun.). Selective inorganic crystalline ion exchange materials for cesium and strontium. United Engineering Foundation and AIChE.

Nyman, M. D., et. al. (1998). CSTs: Stability and use as alternative waste forms. Mat. Res. Soc. Fall Meeting.

Nyman, M. D., et. al. (1999). Hydrothermal synthesis of Cs-Ti-Si-O phases as alternative waste forms for Cs-loaded CST ion exchangers. 1999 Spring American Chemical Society meeting. Anaheim, CA.

Su, Y., et. al. (1998). Evaluation of thermally converted silicotitanate waste forms II. Mat. Res. Soc. Fall Meeting.

Xu, H., et. al. (1999, Apr. 25-28). Thermo-chemistry of crystalline silicotitanate phases in the Cs2O-Na2O-SiO2-TiO2-H2O system. 101st Annual Meeting of the American Ceramic Society. Indianapolis, IN.

Publication Type: Proceeding

Nyman, M. D., et. al. (1998). CSTs: Stability and use as alternative waste forms. Proc. Mat. Res. Soc. Fall Meeting.

Project: 60355

Title: Mineral Surface Processes Responsible for the Decreased Retardation (or Enhanced Mobilization) of ^{137}Cs from HLW Tank Discharges

PI: Dr. John M. Zachara *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Zachara, J. M. (1999, Aug.). New advances in the understanding of 137Cs interactions with micas and implications to Cs geochemistry in the Hanford vadose zone. Keynote address given to the EMSP National Program Workshop. Chicago, IL.

Project: 60387

Title: Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and Misc. Spent Nuclear Fuels

PI: Dr. Denis M. Strachan *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Gu, B. X., Wang, L. M., & Ewing, R. C. (1999, in press). The effect of amorphization on the Cs ion exchange and retention capacity of zeolite-NaY. Journal of Nuclear Materials.

Li, L., Strachan, D. M., Li, H., Davis, L. L., & Qian, M. (1999, in press). Peraluminous and peralkaline effects on Gd2O3 and La2O3 solubilities in sodium-alumino-borosilicate glasses. Ceramic Transactions. American Ceramic Society. Westerville, OH.

Zhao, D., et. al. (1999, in press). Electron microprobe and electron microscopy characterization of precipitated gadolinium crystals in borosilicate glasses. Journal of Non-Crystalline Solids.

Publication Type: Other

Feng, X., et. al. (1999). Distribution and solubility of radionuclides in waste forms for disposition of plutonium and spent nuclear fuels: Preliminary results. In Marra, J. C. & Chandler, G. T. (Eds.), Ceramic Transactions, 93,409-419. American Ceramic Society, Westerville, OH.

Publication Type: Presentation

Davis, L. L., et. al. (1998, Dec.). The effects of Na2O, Al2O3, and B2O3 on HfO2 solubility in borosilicate glass. Materials Research Society, Boston, MA.

Feng, X. (1998, Mar. 17). A plasma arc-vitreous ceramic process for stabilizing EBR-II spent nuclear fuels. National Academy of Science.

Feng, X., et. al. (1998, May). Distribution and solubility of radionuclides in waste forms for disposition of plutonium and spent nuclear fuels: Preliminary results. Symposium of Waste Management Science and Technology in the Ceramic and Nuclear Industries. 100th Am. Cer. Soc. Annual Meeting. Cincinnati, OH.

Li, L., Strachan, D. M., Davis, L. L., Li, H., & Qian, M. (1998, Dec.). Gadolinium solubility limits in sodium-alumino-borosilicate glasses. Materials Research Society Meeting. Boston, MA.

Li, L., Strachan, D. M., Li, H., Davis, L. L., & Qian, M. (1999, Apr. 24-29). Peraluminous and peralkaline effects on Gd2O3 and La2O3 solubilities in sodium-alumino-borosilicate glasses. American Ceramic Society Meeting. Indianapolis, IN.

Shuh, D. K., et. al. (1998, Jul. 28). Distribution and solubility of radionuclides and neutron absorbers in forms for disposition of plutonium ash and scraps, excess plutonium, and miscellaneous spent nuclear fuels. Environmental Management Science Program Workshop Plenary Address. Chicago, IL.

Shuh, D. K., et. al. (1998, Jul. 9). Investigations of actinide materials chemistry utilizing synchrotron radiation methods. Chemical and Analytical Sciences Division, Oak Ridge National Laboratory. Oak Ridge, TN.

Stachan, D. M. (1999, Jun. 1). The Yucca Mountain repository: What has changed? American Geophysical Union, Spring meeting. Boston, MA.

Strachan, D. M. (1999, Apr. 22). Radiation effects in ABO4 orthophosphates and orthosilicates. Invited presentation at theHLW and Pu Immobilization Workshop. CEA, Saclay, France.

Strachan, D. M. (1999, Apr. 5). Performance assessments: The design, selection and importance of nuclear waste forms. Invited presentation at Ch Performance Assessments: The Design, Selection and Importance of Nuclear Waste Forms.

Strachan, D. M. (1999, Jul. 12). Ageing studies of nuclear waste forms: The evaluation of long-term behaviour. Plenary lecture for International Conference on Ageing Studies & Lifetime Extension of Materials, St. Catherine's College. Oxford, United Kingdom.

Strachan, D. M. (1999, Oct. 20). Natural systems: Applications to nuclear waste management. Invited presentation at workshop sponsored by the Russian Academy of Sciences and the U.S. Department of Energy. Moscow, Russia.

Strachan, D. M. (1999, Sept. 10). Radiation effects in zircon. Invited seminar at the Université Henri Poincaré. Nancy, France.

Vance, E. R., et. al. (1999, Apr. 28). Crystal chemistry, radiation effects and aqueous leaching of brannerite, UTi2O6. S-I-059-99, Materials Division, ANSTO, Menai, NSW 2234, Australia.

Publication Type: Proceeding

Davis, L. L., et. al. (1998). The effects of Na2O, Al2O3, and B2O3 on HfO2 solubility in borosilicate glass. In Scientific Basis for Nuclear Waste Management XXII. Materials Research Society. Pittsburgh, PA.

Ewing, R. C. (1999, in press). Ageing studies of nuclear waste forms: The evaluation of long-term behaviour. Proceedings of International Conference on Ageing Studies & Lifetime Extension of Materials.

Li, L., Strachan, D. M., Davis, L. L., Li, H., & Qian, M. (1998). Gadolinium solubility limits in sodium-alumino-borosilicate glasses. In Scientific Basis for Nuclear Waste Management XXII, Materials Research Society. Pittsburgh, PA.

Strachan, D. M. (1999, Nov. 13). Mineralogy: Applications to nuclear waste disposal. Plenary presentation at the Twentieth Annual New Mexico Mineral Symposium, New Mexico Institute of Mining and Technology. Socorro, NM.

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999). Electron irradiation of zeolites. In Zinkle, S. J., Lucas, G. E., Ewing, R. C., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Symposium Proceedings of the Materials Research Society, 540,361-366.

Project: 60392

Title: Radiolytic and Thermal Process Relevant to Dry Storage of Spent Nuclear Fuels

PI: Dr. Steven C. Marschman *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Petrik, N. G., Alexandrov, A. B., Vall, A., & Orlando, T. M. (1999, in press). Gamma radiolysis of water on oxide surfaces: Parameters controlling the energy transfer.

Petrik, N. G., Taylor, D. P., & Orlando, T. M. (1999). Laser-stimulated luminescence of yttria-stabilized cubic-zirconia crystals. J. Appl. Phys. 85,6770.

Simpson, W. C., Wang, W. K., Yarmoff, J. A., & Orlando, T. M. (1999). Photon- and electron-stimulated desorption of O + from zirconia. Surf. Sci., 423,225.

Publication Type: Presentation

Haustein, P. (1999, Aug. 22-26). Nuclear stimulated desorption at the surfaces of model SNF materials: Experiment and computer simulation. Invited presentation at the Annual Symposium on First Accomplishments of the Environmental Management Science Program, American Chemical Society. New Orleans, LA.

Hedhili, M. N., Yakshinskiy, B. V., & Madey, T. E. (1999, Mar. 21-25). Interaction of water with UO2 (001). National American Physical Society Meeting. Atlanta, GA.

Hedhili, M. N., Yakshinskiy, B. V., Madey, T. E., Dobrozemsky, R., & Yarmoff, J. (1999, Aug. 22-26). Interaction of water with uranium oxide surfaces. Annual Symposium on First Accomplishments of the Environmental Management Science Program. American Chemical Society. New Orleans, LA.

Orlando, T. M. (1999, Mar. 21-25). Quantum-resolved studies of condensed phase reactions. Invited presentation at the Annual Meeting of the Symposium on Free radicals in the Condensed Phase. American Chemical Society. Anaheim, CA.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 24). Nonthermal processes on oxide surfaces and interfaces. Invited presentation at the Los Alamos National Laboratory. Los Alamos, NM.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 24-25). Nonthermal processes on oxide surfaces and interfaces. DOE Laboratory Catalysis Research Symposium. Albuquerque, NM.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 26). Nonthermal processes on oxide surfaces and interfaces. Invited presentation at the Department of Chemistry, University of Utah. Salt Lake City, UT.

Orlando, T. M., Petrik, N., Marshman, S., & Camaioni, D. M. (1999, Nov. 14-18). Nonthermal surface processes in the generation of gas in mixed wastes. Invited presentation at the Annual Meeting of the American Nuclear Society. Long Beach, CA.

Petrik, N., Marshman, S., Camaioni, D. M., & Orlando, T. M. (1999, Aug. 22-26). Nonthermal surface and interface processes in the storage of spent nuclear fuel and mixed wastes. Annual Symposium on First Accomplishments of the Environmental Management Science Program. American Chemical Society. New Orleans, LA.

Project: 60451

Title: Mechanics of Bubbles in Sludges and Slurries
PI: Dr. Phillip A. Gauglitz *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Kam, S. I. & Rossen, W. R. (1999, in press). Anomalous capillary pressure, stress and stability of solids-coated bubbles. J. Colloid Interface Sci.

Publication Type: Presentation

Gauglitz, P. A., et. al. (1998, Jun.). Mechanics of bubbles in sludges and slurries: Initial progress. Hanford Technical Exchange. Richland, WA.

Gauglitz, P. A., et. al. (1999, Jan.). Mechanics of bubbles in sludges and slurries. Presented at the Hanford Site Technology Coordinating Group - Tank Subgroup. Richland, WA.

Gauglitz, P. A., Terrones, G., Aardahl, C. L., Mendoza, D. P., & Mahoney, L. A. (1999, Mar. 14-19). Mechanics of bubbles in sludges and slurries: Experi-mental studies and solid mechanics modeling results. Engineering Founda-tion Conference on Rheology in the Minerals Industry II. Oahu, HI.

Publication Type: Report

Kam, S. I. (1998). Interactions between bubbles and solids: Three applications. Department of Petroleum and Geosystems Engineering. The University of Texas, Austin, TX.

Project: 60474

Title: Ultrahigh Sensitivity Heavy Noble Gas Detectors for Long-Term Monitoring and Monitoring Air

PI: Dr. John D. Valentine *Institution:* Georgia Institute of Technology

Publication Type: Journal

Valentine, J. D. (1999). Evaluating detectors and pulse processing techniques. IEEE Transactions in Nuclear Science, 46(3).

Publication Type: Other

Valentine, J. D. (1999). Small prototype fluid transfer system and its performance. Nuclear Instruments and Methods in Physics Research, Section A, 422,820-825.

Project: 64907

Title: "Green" Biopolymers for Improved Decontamination of Metals from Surfaces: Sorptive Characterization and Costing Properties

PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

Publication Type: Poster

Davison, B. H. (1998, Nov. 17-18). Green biopolymers for decontamination. Poster presentation at Workshop on integration of end user needs with research projects for EMSP: Focus on Deactivation and Decommissioning at Savannah River Site.

Publication Type: Presentation

Davison, B. H. (1999, Sept. 12-17). Green biopolymer for decon of contaminated surfaces. Decontamination, Demolition, and Restoration (DD&R) Topical Meeting on Site Restoration of Government and Commercial Facilities. Knoxville, TN.

Project: 64946

Title: Mechanisms of Radionuclide-Hydroxycarboxylic Acid Interactions for Decontamination of Metallic Surfaces

PI: Dr. A.J. Francis *Institution:* Brookhaven National Laboratory

Publication Type: Presentation

Halada, G. P., et. al. (1999, May 2-6). Interaction of uranium with corrosion products formed on plain carbon steel. Paper presentation at the 195th Meeting of the Electrochemical Society. Seattle, WA.

Publication Type: Proceeding

Francis, A. J., Dodge, C. J., Gillow, J. B., Halada, G. B., & Clayton, C. R. (1999, Aug. 22-26). Decontamination of uranium contaminated metallic surfaces with uranium recovery. Paper presentation NUCL-65 at the Symposium on First Accomplishments of Environmental Management Science Program, 218th Annual Meeting of the American Chemical Society. New Orleans, LA.

Halada, G. P., et. al. (1999, Aug. 22-26). A spectroscopic study of the association of contaminant uranium with mild steel corrosion products. Paper presentation NUCL-61at the Symposium on First Accomplishments of Environmental Management Science Program, 218th Annual Meeting of the American Chemical Society. New Orleans, LA.

Project: 64965

Title: Supercritical Carbon Dioxide-Soluble Ligands for Extracting Actinide Metal Ions from Porous Solids

PI: Dr. Mark L. Dietz *Institution:* Argonne National Laboratory

Publication Type: Poster

Herlinger, A. W., Griffith, J. A., McAlister, D. R., & Barrans Jr., R. E. (1999, Aug. 22-26). Functionalized diphosphonic acid ligands for metal ion coordination in supercritical carbon dioxide. Poster presentation #33 at the First Accomplishments of the Environmental Management Sciences Program Symposium sponsored by the Division of Nuclear Chemistry and Technology at the 218th National A.C.S. Meeting. New Orleans, LA.

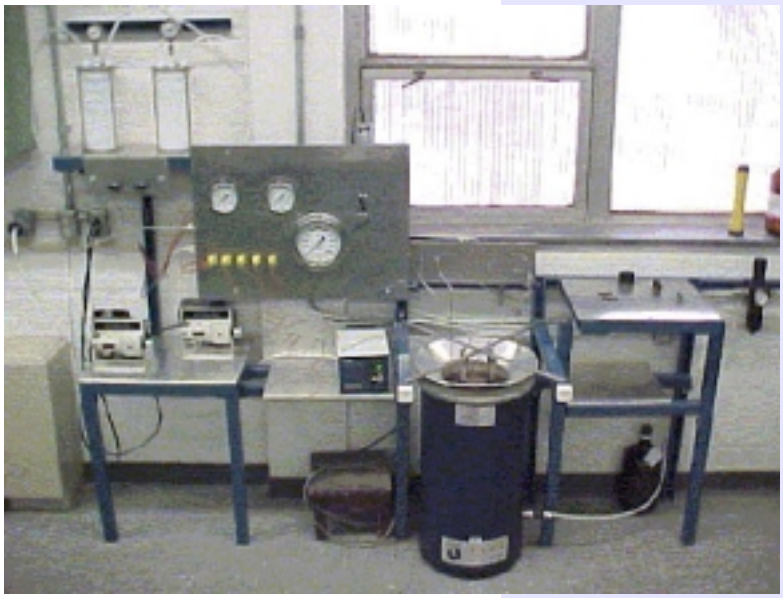
Project: 64979

Title: Decontamination and Decommissioning of PCB Sites at DOE: Extraction, Electrokinetics, and Hydrothermal Oxidation

PI: Dr. Edward A. Hamilton
Institution: SCUREF

Publication Type: Poster

Pickett, J., et. al. (1998, Nov. 17-18). Decontamination & decommissioning of PCB sites at SRS. Poster presentation at the Workshop on Integration of End User Needs with Research Projects for the Environmental Management Science Program. Savannah River Site. Aiken, SC.



Supercritical Water Oxidation Test Stand at Clemson University. [see Project #64979]

Publication Type: Presentation

Bruce, D. (1998, Nov. 15-20). Sonochemical oxidation of organic contaminants in waste water. Presentation at the AIChE Annual Meeting. Miami Beach, FL.

Matthews, M. (1998, Nov. 15-20). Mass transfer in CO2/surfactant systems. Presentation at the 1998 AIChE Annual Meeting. Miami Beach, FL.

Project: 65001

Title: Development of Novel, Simple Multianalyte Sensors for Remote Environmental Analysis

PI: Dr. Sanford A. Asher *Institution:* University of Pittsburgh

Publication Type: Journal

Holtz, J. H. & Asher, S. A. (1997). Intelligent polymerized crystalline colloidal array hydrogel film chemical sensing materials. Nature, 389,829-832.

Holtz, J. H., Holtz, J. S. W., Munro, C. H., & Asher, S. A. (1998). Intelligent polymerized crystalline colloidal arrays: Novel chemical sensor materials. Anal. Chem., 70,780-791.

Holtz, J., Weissman, J., Pan, G., & Asher, S. A. (1998). Mesoscopically periodic photonic crystal materials for linear and nonlinear optics and chemical sensing. Material Research Soc., 23,44-50.

Project: 65004

Title: Real-Time Identification and Characterization of Asbestos and Concrete Materials with Radioactive Contamination

PI: Dr. George Xu *Institution:* Rensselaer Polytechnic Institute

Publication Type: Journal

Naessens, E. P. & Xu, X. G. (1999). A non-destructive method to determine the depth of radionuclides in materials in-situ. Health Physics, 77(1),76-88.

Publication Type: Presentation

Chen, Q., Jiang, Z., Sun, F. G., & Zhang, X. -C. (1999, May). Two-fold improvement of THz optoelectronic generation and detection. CLEO'99. Baltimore, MD.

Jiang, Z., Sun, F. G., Chen, Q., & Zhang, X. -C. (1999, May). Electro-optic sampling near zero optical transmission point. CLEO'99. Baltimore, MD.

Project: 65352

Title: Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation

PI: Dr. Sue B. Clark *Institution:* Washington State University

Publication Type: Journal

Clark, S. B. (1999, in press). The aqueous geochemistry of the rare earth elements. IX. A potentiometric study of Nd 3+ complexation with acetate in 0.1 molal NaCl solutions from 25-225° C. Geochim. Cosmochim. Acta.

Publication Type: Paper

Wood, S. A., Palmer, D. A., Wesolowski, D. J. (1999, Aug. 22-27). Determination of the solubility of crystalline Nd(OH)3 in sodium triflate solutions from 30 to 250 C with in situ pH measurement. Determination of the solubility of crystalline Nd(OH)3 in sodium triflate solutions from 30 to 250 C with in situ pH measurement. Ninth Annual V.M. Goldschmidt Conference Abstracts. Harvard University, Cambridge, MA. Lunar and Planetary Institute Contribution No. 791. Houston, TX. 329-330.

Project: 65366

Title: Physical, Chemical and Structural Evolution of Zeolite-Containing Waste Forms Produced From Metakaolinite and Calcined HLW

PI: Dr. Michael W. Grutzeck *Institution:* Pennsylvania State University

Publication Type: Proceeding

Siemer, D. D., Grutzeck, M. W., & Scheetz, B. E. (1999, Apr. 25-28). Comparison of materials for making hydroceramic waste forms. Proc. Amer. Ceram. Soc. Symposium on Waste Management Science and Technology in the Ceramic and Nuclear Industries, Indianapolis, IN. American Ceramic Society. Westerville, OH.

Project: 65370

Title: Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics

PI: Dr. Glen E. Fryxell *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Feng, X., et. al. (1999). Self-assembled monolayers on mesoporous silica, a super sponge for actinides. In Mara, J. C. & Chandler, G. T. (Eds.), Ceramic Transactions, 93, Environmental Issues and Waste Management Technologies IV, 35-42.

Fryxell, G. E., et. al. (1999, in press). Design and synthesis of selective mesoporous anion traps. Chemistry of Materials.

Publication Type: Other

Fryxell, G. E. & Liu, J. (1999, in press). Designing surface chemistry in mesoporous silica. In Papirer, E. (Ed.), Adsorption at Silica Surfaces. Marcel Dekker.

Publication Type: Presentation

Fryxell, G. E., et al. (1999, Jun.). Self-assembled monolayers on mesoporous supports: Synthesis of nanoscale hybrid materials and their applications. Presentation at the Northwestern Regional Meeting of the American Ceramic Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Apr.). Design and synthesis of mesoporous lanthanide sorbent materials. Invited presentation at the 101st National Meeting of the American Ceramic Society.

Fryxell, G. E., et. al. (1999, Apr.). Environmental applications of interfacially modified mesoporous ceramics. Invited presentation at the 101st National Meeting of the American Ceramic Society.

Fryxell, G. E., et. al. (1999, Aug.). Environmental applications of Self-Assembled Monolayers on Mesoporous Supports (SAMMS). Invited presentation at the National Meeting of the American Ceramic Society. New Orleans, LA.

Fryxell, G. E., et. al. (1999, Jun.). High efficiency environmental sorbent materials: Self-assembled Monolayers on Mesoporous Support (SAMMS) for metal removal from aqueous systems. Presentation at the Symposium on Environmental Chemistry at the Northwestern Regional Meeting of the American Chemical Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Jun.). High efficiency environmental sorbent materials: Self-assembled Monolayers on Mesoporous Supports (SAMMS) for metal removal from aqueous systems. Presentation at the Northwestern Regional Meeting of the American Ceramic Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Jun.). Self assembled monolayers on mesoporour supports: Synthesis of nanoscale hybrid materials and their applications. Presentation at the Symposium on Nanoscale Materials at the Northwestern Regional Meeting of the American Chemical Society. Portland, OR.

Publication Type: Press release

Fryxell, G. E. (1999, Apr. 11). PNNL focuses on healthy environment. Tri-City Herald, D1.

Fryxell, G. E. (1999, Mar.). Metal eaters. Popular Science, 34.

Project: 65371

Title: Numerical Modeling of Mixing of Chemically Reacting, Non-Newtonian Slurry for Tank Waste Retrieval
PI: Dr. David A. Yuen *Institution:* University of Minnesota

Publication Type: Journal

Ten, A. A., Podladchikov, Y. Y., Yuen, D. A., Larsen, T. B., & Malevsky, A. V. (1998). Comparison of mixing properties in convection with the particle-line method. Geophys. Res. Lett., 25(16),3205-3208.

Ten, A. A., Yuen, D. A. & Podladchikov, Y. Y. (1999, in press). Numerical modeling of mixing of chemically reacting, non-Newtonian slurry for tank waste retrieval. Electronic Geosciences.

Publication Type: Presentation

Onishi, Y., Trent, D. S., Michener, T. E., Van Beek, J. E., & Rieck, C. A. (1999, Jul. 18-23). Simulation of radioactive tank waste mixing with chemical reactions. FEDSM99-7786, presentation at the 3rd ASME/JSME Joint Fluids Engineering Conference. San Francisco, CA.

Publication Type: Proceeding

Onishi, Y. & Trent, D. S. (1999, Mar. 14-19). Mobilization modeling of erosion-resisting radioactive tank waste. Proceedings of Rheology in the Mineral Industry II, Kahuku, Oahu, HI. Organized by United Engineering Foundation. New York, NY. 45-56.

Onishi, Y., Trent, D. S., Michener, T. E., Van Beek, J. E., & Rieck, C. A. (1999, Jul. 18-23). Simulation of radioactive tank waste mixing with chemical reactions. FEDSM99-7786: Proceedings of 3rd ASME/JSME Joint Fluids Engineering Conference. San Francisco, CA.

Project: 65408

Title: Mechanisms and Kinetics of Organic Aging in High-Level Nuclear Wastes
PI: Dr. Donald M. Camaioni *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Autrey, S. T. (1999, Apr. 30). Nitrosyl transfer reactions are not catalyzed by Al(OH)4. Notre Dame Radiation Laboratory and Pacific Northwest National Laboratory EEMSP Coordination Meeting and Technical exchange. Notre Dame, IN.

Camaioni, D. M. (1998, Nov. 17). Mechanisms and kinetics of organic aging in high level wastes. EMSP/Tanks Focus Area Workshop. Richland, WA.

Camaioni, D. M. (1998, Oct. 29). Mechanisms and kinetics of the degradation of organic complexants in nuclear waste. Chemistry Seminar, Notre Dame Radiation Laboratory. Notre Dame, IN.

Camaioni, D. M. (1999, Aug. 22-26). Thermochemical kinetic analysis of thermal pathways for oxidation of organic complexants in high level wastes. First Accomplishments of the Environmental Management Science Program. Annual Meeting of the American Chemical Society. New Orleans, LA.

Project: 65410

Title: Rapid Migration of Radionuclides Leaked from High-Level Waste Tanks: A Study of Salinity Gradients, Wetted Path Geometry and Water Vapor Transport

PI: Dr. Anderson L. Ward *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Selker, J. S. (1998, Dec. 5-10). Fingered flow from high salinity sources. Presented at the AGU Fall Meetings. San Francisco, CA.

Ward, A. L. & Gee, G. W. (1999, Oct. 31 - Nov. 4). A numerical analysis of wetting front instability induced by infiltration of highly saline fluids. Symposium on Preferential Flow, Soil Science Society of America Annual Meeting. Salt Lake City, UT.

Project: 65421

Title: Correlation of Chemisorption and Electronic Effects for Metal/Oxide Interfaces: Transducing Principles for Temperature-Programmed Gas Microsensors

PI: Dr. Stephen Semancik *Institution:* National Institute of Standards & Technology

Publication Type: Presentation

Cavicchi, R. E. (1998, Nov. 17). Correlation of chemisorption and electronic effects for metal/oxide interfaces: Transducing principles for temperature programmed gas microsensors. Environmental Management Science Program - Tank Focus Area Workshop. Richland, WA.

Cavicchi, R. E. (1999, Sept. 17-22). Microhotplate gas sensor arrays. Presentation at the SPIE International Symposium on Environmental and Industrial Sensing. Boston, MA.

Ding, J. (1999, Sept. 17-22). Quantification of a single component gas in air with a microhotplate gas sensor using partial least squares techniques. Presentation at the SPIE International Symposium on Industrial and Environmental Sensing. Boston, MA.

McAvoy, T. J. (1999, Aug. 24). Modeling microhotplate gas sensors. Presentation at the ACS National Meeting. New Orleans, LA.

Panchapakesan, B. (1999, Apr. 7). Micromachined array studies of tin oxide films: Nucleation, structure and gas sensing characteristics. MRS Spring National Meeting. San Francisco, CA.

Semancik, S. (1999, Aug. 24). Microarrays as platforms for gas microsensor development and efficient materials research. Presentation at the ACS National Meeting. New Orleans, LA.

Semancik, S. (1999, Sept.). Solid state gas microsensors for environmental and industrial monitoring. Presentation at the SPIE International Symposium on Industrial and Environmental Sensing. Boston, MA.

Walton, R. M. (1999, Jun. 7). Processing methods for selected area film deposition and preparation on microsensor platforms using thermal and potential control. 10th International Conference on Solid-State Sensors and Actuators. Sendai, Japan.

Publication Type: Proceeding

Panchapakesan, B., DeVoe, D. L., Cavicchi, R. E., Walton, R. M., & Semancik, S. (1999, in press). Micromachined array studies of tin oxide films: Nucleation, structure and gas sensing characteristics. Proceedings of the MRS, Spring 1999.

Walton, R., et. al. (1999, Jun.). Processing methods for selected area film deposition and preparation on microsensor platforms using thermal and potential control. Digest 10th International Conference on Solid-State Sensors and Actuators, 1,676-679. Sendai, Japan.

Project: 65422

Title: Modeling of Spinel Settling in Waste Glass Melter
PI: Dr. Pavel Hrma *Institution:* Pacific Northwest National Laboratory

Publication Type: Paper

Hrma, P. (1999). Spinel precipitation in high-level waste glass. Proceedings of the 5th ESG Conference. Prague, Czechoslovakia.

Project: 65425

Title: Mass Spectrometric Fingerprinting of Tank Waste Using Tunable, Ultrafast Infrared Lasers
PI: Dr. Richard F. Haglund,Jr. *Institution:* Vanderbilt University

Publication Type: Presentation

R. F. Haglund, Jr., (1999, Jun.). The future of tunable, ultrafast lasers in materials analysis and processing. Plenary Lecture at the American Society for Mass Spectrometry. Dallas, TX.

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